Supporting Information

Macrocyclic Diorganotin Complexes of γ-Amino Acid Dithiocarbamates as Hosts for Ion-Pair Recognition

Jorge Cruz-Huerta,[a] Manuel Carillo-Morales,[a] Ericka Santacruz-Juárez,[a] Irán F. Hernández-Ahuactzi,[a] Jaime Escalante-García,[a] Carolina Godoy-Alcantar,[a] Jorge A. Guerrero-Alvarez,[a] Herbert Höpfl,[a,*] Hugo Morales-Rojas,[a] Mario Sánchez[b]

[a)] Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos, Av. Universidad 1001, C.P. 62209 Cuernavaca, México. E-mail: hhopfl@ciq.uaem.mx. [b)] Facultad de Química, Universidad de Guanajuato, Noria Alta s/n, C.P. 36050 Guanajuato, México.

Preparation and spectroscopic data of ligands **L2** and **L3**

* Corresponding author. Fax: (+52) 777 329 79 97
E-mail address: hhopfl@ciq.uaem.mx (H. Höpfl)

a solution in $CDCl_3$ at 25 ^oC. The solid curve is fitting to a 1:1 binding model from which K_{as} was calculated.

Table S1. Atomic coordinates and selected geometric parameters for the calculated molecular structure of compound **5** (B3LYP/SBKJC(d,p)).

Table S2. Calculated and experimental vibrational frequencies for $[Me_2Sn(\mathbf{L3}\text{-dtc})]_3$ (**5**).

Table S3. Selected NMR spectroscopic data for compounds **L1**·HCl, **L2**, **L3** and **1**-**7** (in $CDCl_3$, ppm).

Table S4. Atomic coordinates and selected geometric parameters for the calculated molecular structure of compound **1** (B3LYP/SBKJC(d,p)).

Preparation and spectroscopic data of ligands L2 and L3

3-(Benzylamino)propionic acid **L2**

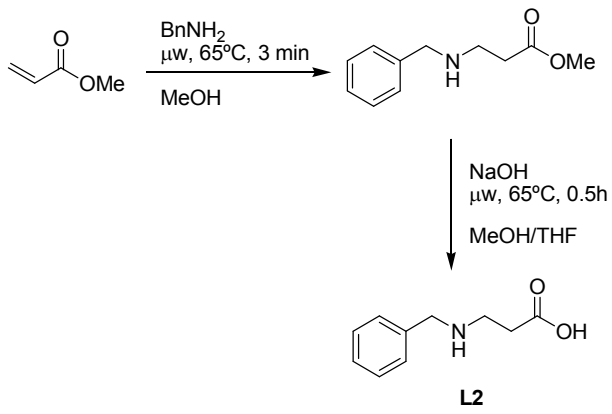
Benzylamine (3.60 g, 33.6 mmol), methyl acrylate (3.18 g, 36.9 mmol) and methanol (10 mL) were reacted by microwave heating to 65 °C for 10 min to afford methyl 3-(benzylamino) propionoate, which was purified by column chromatography on silica, eluting with hexane-ethyl acetate (8:2). Yield: 5.30 g, 82 %. ^{1}H-NMR (200 MHz, $CDCl_3$, 20 ºC, TMS): δ = 1.82 (br s, 1H, CH_2-*NH*-CH_2), 2.54 (t, J = 6.6 Hz, 2H, CH_2-*CH_2*-COO), 2.89 (t, J = 6.4 Hz, 2H, *CH_2*-CH_2-COO), 3.67 (s, 3H, O*CH_3*), 3.80 (s, 2H, C_6H_5-*CH_2*), 7.29-7.42 (m, 5H, *C_6H_5*) ppm. ^{13}C-NMR (50 MHz, $CDCl_3$, 20 ºC, TMS): δ = 34.7 (CH_2-*CH_2*-COO), 44.6 (*CH_2*-CH_2-COO), 51.8 (C_6H_5-*CH_2*-N), 53.9 (O*CH_3*), 127.0, 128.1, 128.5 (*o*-C_6H_5, *m*-C_6H_5, *p*-C_6H_5), 140.0 (*i*-C_6H_5), 173.2 (COO) ppm.

Methyl 3-(benzylamino) propionoate (5.60 g, 29 mmol) was hydrolyzed with NaOH (2.60 g, 65 mmol) in MeOH/THF (10 mL) by microwave heating to 75 ºC for 1 h (according to TLC). After evaporation of the solvent under reduced pressure, the residue was acidified with aqueous 1N HCl until the solution reached pH 2. The resulting chlorohydrate was passed through an ion-exchange resin column (DOWEX-50WX8-200) to afford **L2** as a white solid. Yield: 4.40 g, 84 %. Mp: 174-176 ºC. ^{1}H-NMR (400 MHz, D_2O, 20 ºC): δ = 2.48 (t, J = 6.8 Hz, 2H, CH_2-*CH_2*-COO), 3.12 (t, J = 7 Hz, 2H, *CH_2*-CH_2-COO), 4.14 (s, 2H, C_6H_5-*CH_2*-N), 7.40-7.41 (m, 5H, *C_6H_5*) ppm. ^{13}C-NMR (100 MHz, D_2O, 20 ºC): δ = 32.5 (CH_2-*CH_2*-COO), 43.9 (*CH_2*-CH_2-COO), 50.8 (C_6H_5-*CH_2*), 129.3, 129.6, 129.7 (*o*-C_6H_5, *m*-C_6H_5, *p*-C_6H_5), 130.7 (*i*-C_6H_5), 177.8 (COO) ppm.

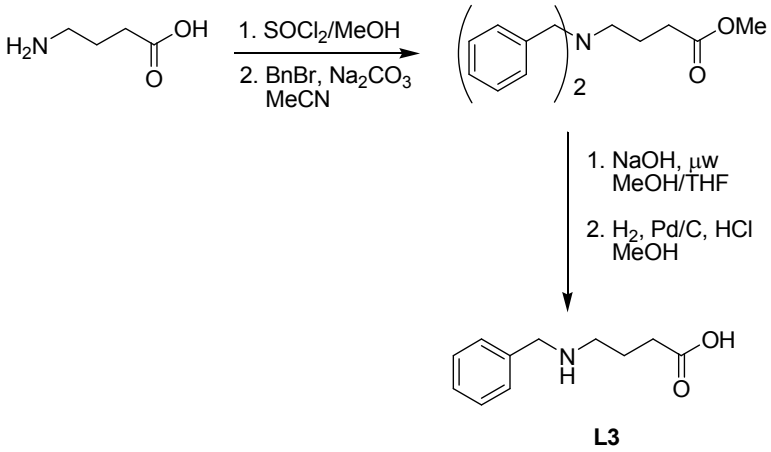
4-(benzylamino)butyric acid ***L3***

To a solution of 4-aminobutyric acid (1.00 g, 9.7 mmol) in MeOH (15 ml) at 0 ºC, $SOCl_2$ (1.70 g, 14.6 mmol) was added. After stirring the solution for 1.5 h, it was allowed to reach room temperature, whereupon the solvent was evaporated to obtain methyl 4-amino butyrate as yellow oil (1.13 g, quantitative, identified by ^{1}H NMR). The β-amino ester (1.13 g, 9.7 mmol) was dissolved in acetonitrile (25 mL) and benzyl bromide (3.70 g, 21.6 mmol) was added. After cooling the solution to 0 ºC and addition of Na_2CO_3 (2.31 g, 22 mmol), the resultant mixture was stirred for 24 h at room temperature. Then, the solvent was evaporated and the reaction mixture extracted with ethyl acetate (3 x 15 mL). The organic phase was dried with $MgSO_4$ and evaporated under reduced pressure. The crude was purified by column

chromatography (hexane: ethyl acetate, 8:2 → 5:5) to produce methyl 4-(dibenzylamino) butyrate as a viscous yellow oil. Yield: 1.45 g, 50 %. ^{1}H-NMR (200 MHz, CD_3OD, 20 ºC, TMS): δ = 1.76 (q, J = 7 Hz, 2H, CH_2-*CH_2*-CH_2), 2.27 (t, J = 7.1 Hz, 2H, CH_2-*CH_2*-COO), 2.38 (t, J = 6.8 Hz, 2H, N-*CH_2*-CH_2), 3.48 (s, 4H, C_6H_5-*CH_2*-N), 3.54 (s, 3H, O*CH_3*), 7.19-7.33 (m, 10H, *C_6H_5*) ppm. ^{13}C-NMR (50 MHz, CD_3OD, 20 ºC, TMS): δ = 23.4 (CH_2-*CH_2*-CH_2), 32.5 (CH_2-*CH_2*-COO), 52.1, 53.4 (N-*CH_2*-CH_2, O*CH_3*), 59.4 (C_6H_5-*CH_2*-N), 128.0, 129.3, 130.0 (*o*-C_6H_5, *m*-C_6H_5, *p*-C_6H_5), 140.8 (*i*-C_6H_5), 175.7 (COO) ppm. For the preparation of *4-(benzylamino)butyric acid* **L3**, to a solution of methyl 4-(dibenzylamino) butyrate (1.90 g, 6.4 mmol) in MeOH/THF (20 mL), an aqueous solution of NaOH (0.90 g, 22.6 mmol) was added. The reaction mixture was microwave- heated to 65 ºC for 0.5 h. After evaporation of the solvent under reduced pressure, the residue was dissolved in H_2O and acidified with aqueous 1N HCl until it reached pH 3. The acidic solution was then evaporated under vacuum and the residue was redissolved in MeOH, whereby insoluble salts were separated by filtration. After removal of the solvent by vaccum distillation, the monohydrogenolysis reaction was carried out without further purification. Pd/C catalyst (0.30 g, 15% w/w) and 2-3 drops of concentrated HCl were added, and then the reaction mixture was stirred and pressurized with H_2 (60 lb) for 2h. After filtration of the mixture and concentration under reduced pressure, the crude product was passed through an ion-exchange resin column (DOWEX-50WX8-200) to afford 4-(benzylamino)butyric acid **L3** as white solid. Yield: 0.95 g, 77 %. Mp: 129-131 ºC. ^{1}H-NMR (400 MHz, CD_3OD, 20 ºC, TMS): δ = 1.88 (q, J = 6.4 Hz, 2H, CH_2-*CH_2*-CH_2), 2.35 (t, J = 6.6 Hz, 2H, CH_2-*CH_2*-COO), 3.06 (t, J = 6.4 Hz, 2H, NH_2-*CH_2*-CH_2), 4.14 (s, 2H, C_6H_5-*CH_2*-NH), 7.41–7.50 (m, 5H, *C_6H_5*) ppm. ^{13}C NMR (100 MHz, CD_3OD, 20 ºC, TMS): δ = 23.6 (CH_2-*CH_2*-CH_2), 37.2 (CH_2-*CH_2*-COO), 49.3 (N-*CH_2*-CH_2), 52.1 (Ph-*CH_2*-N), 130.2, 130.4, 130.7 (*o*-C_6H_5, *p*-C_6H_5, *m*- C_6H_5), 133.4 (*i*- C_6H_5), 180.9 (COO) ppm.

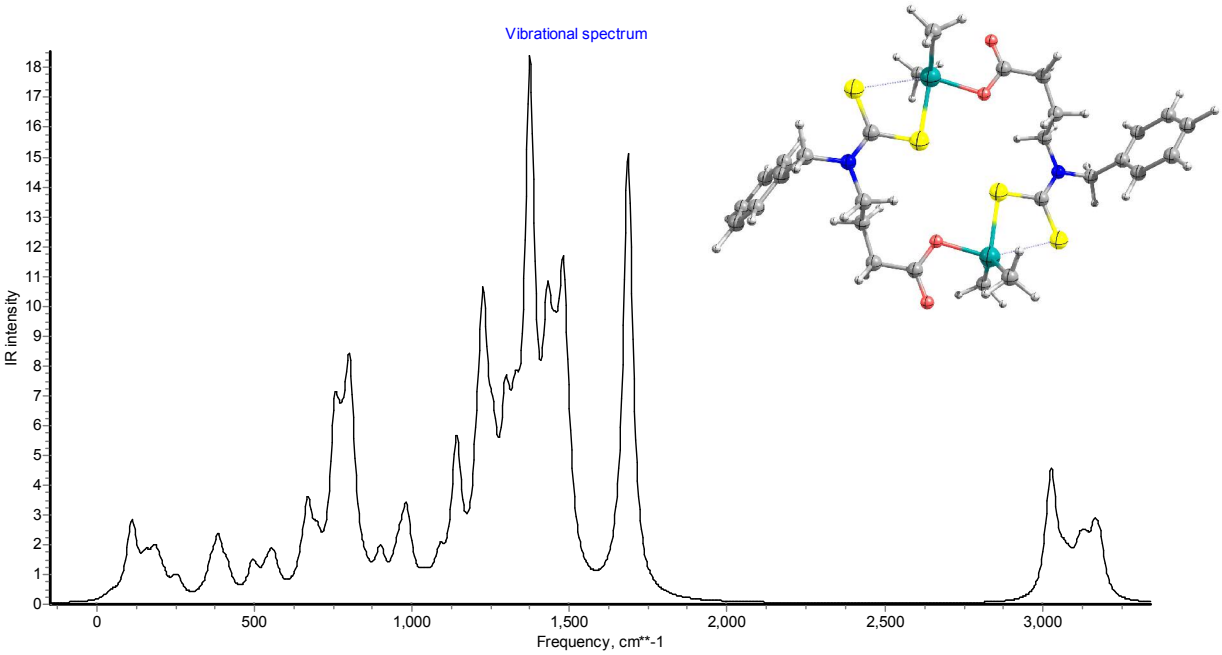


Scheme S1. Synthesis of 3-(benzylamino)propionic acid **L2**.



Scheme S2. Reaction sequence for the benzylation of 4-aminobutyric acid.

a)



b)

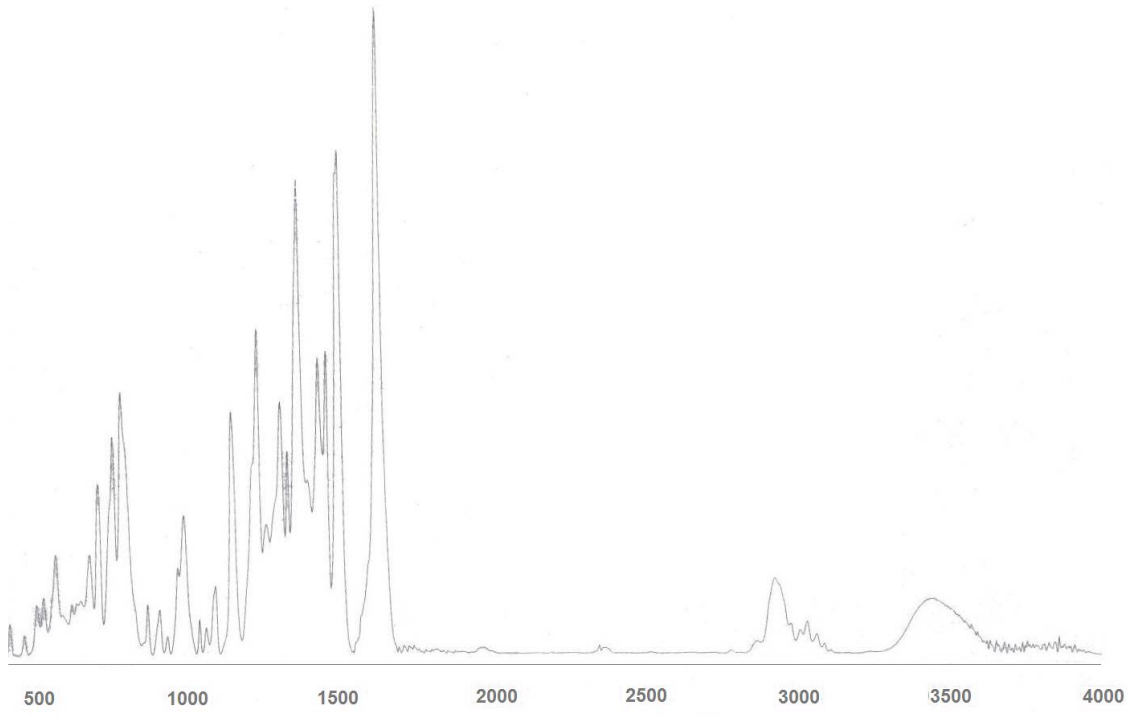


Figure S1. Calculated (B3LYP/SBKJC(d,p)) and experimental (KBr) IR spectra for compound **5**.

a)

b)

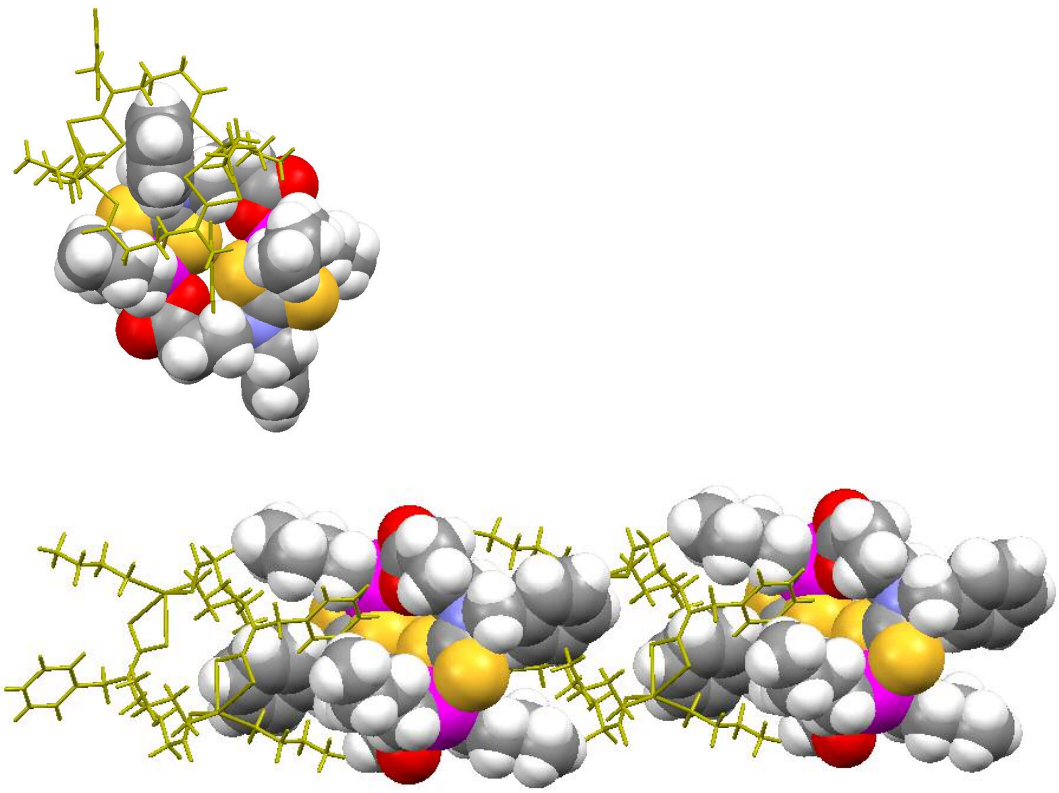


Figure S2: Perspective view of the supramolecular synthon (a) in the crystal structure of compound **6** that gives rise to 1 1D molecular arrangement (b).

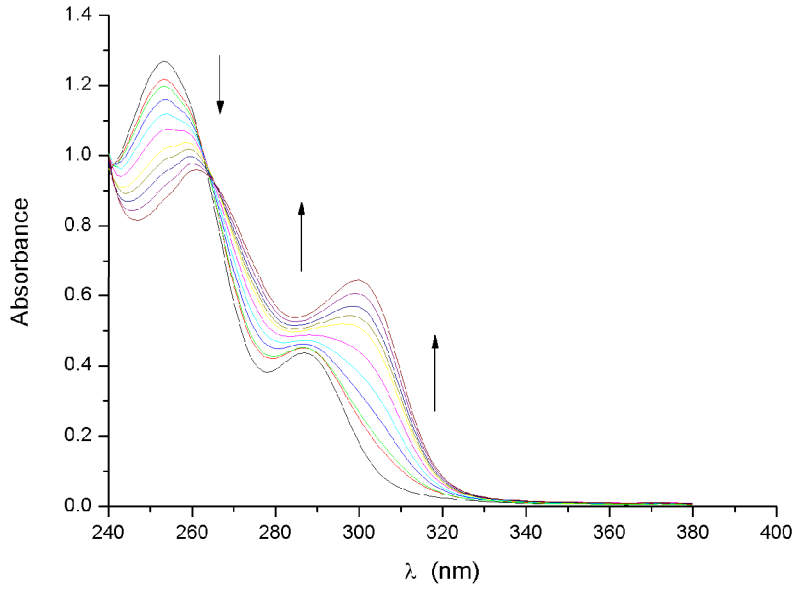


Figure S3. Changes of the absortion spectra during the titration of **7** (6.7 x 10^{-5} M) with different quantities of AcOTBA (0 - 3.6 x10^{-2} M) in $CHCl_3$. The arrows indicate the spectral changes occurring in response to an increasing concentration of AcOTBA.

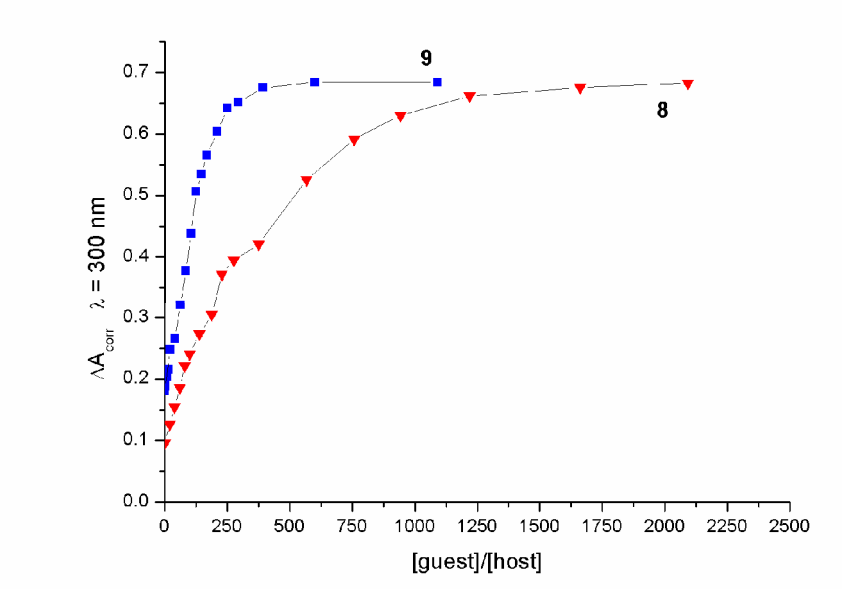


Figure S4. Plots for the titration of compounds **8** and **9** with AcOTBA in $CHCl_3$.

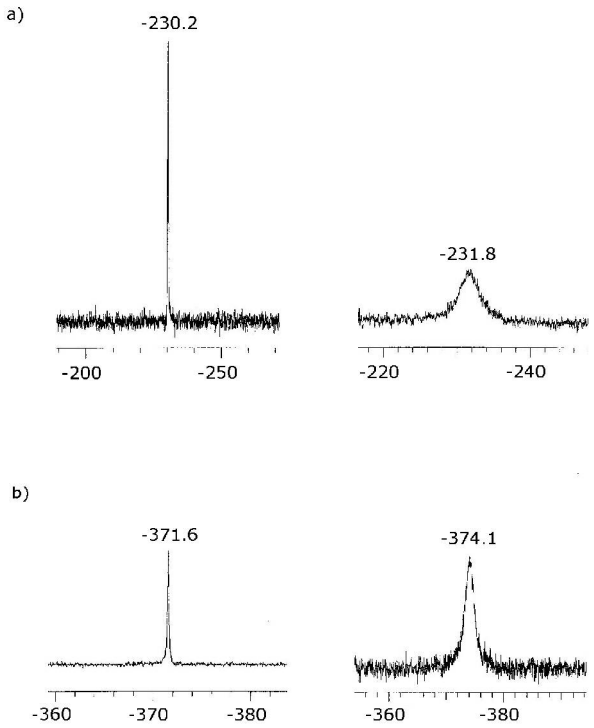


Figure S5. ^{119}Sn NMR spectra before and after addition of AcOTBA for compounds a) **6** and b) **7**.

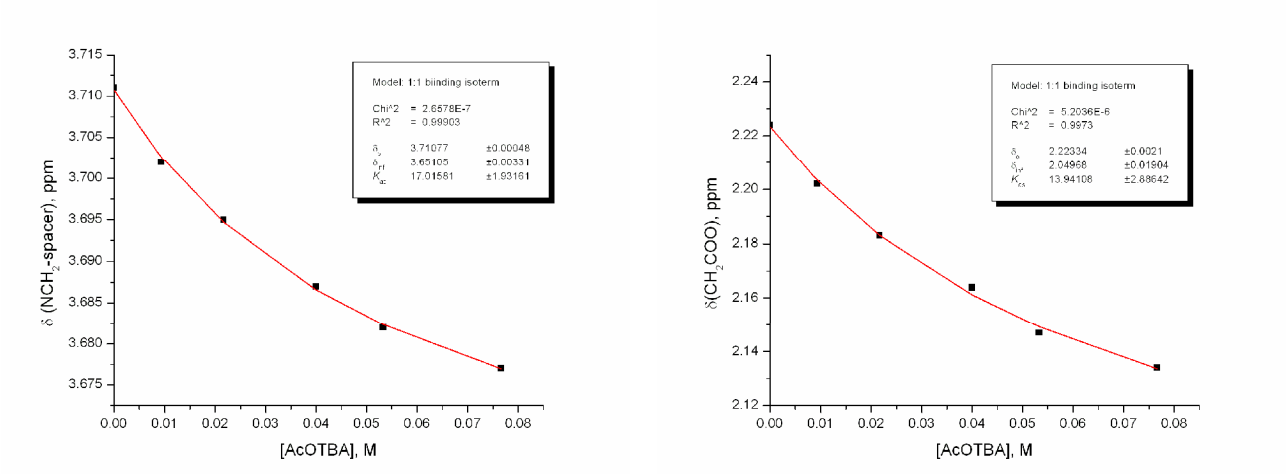


Figure S6. Complexation induced shifts (CIS) for the ^{1}H NMR signals of the N-C*H*$_2$-spacer (left) and C*H*$_2$-COO groups (right) in compound **6** upon addition of AcOTBA in a solution in $CDCl_3$ at 25 ^{o}C. The solid curve is fitting to a 1:1 binding model from which K_{as} was calculated.

Table S4. Atomic coordinates and selected geometric parameters for the calculated molecular structure of compound **5** (B3LYP/SBKJC(d,p)).

Sn	1.121192963	-3.368859326	-0.027920088
Sn	-1.121192963	3.368859326	0.027920088
S	1.558718431	-0.956712670	0.523235715
S	-1.558718431	0.956712670	-0.523235715
S	3.915305880	-2.822920204	0.411776889
S	-3.915305880	2.822920204	-0.411776889
N	4.087245497	-0.186715003	1.068805928
N	-4.087245497	0.186715003	-1.068805928
O	-0.904109640	-2.757316989	-0.002171278
O	0.904109640	2.757316989	0.002171278
O	-1.285646932	-4.893992493	-0.605544418
O	1.285646932	4.893992493	0.605544418
C	3.301326450	-1.229987138	0.703444161
C	-3.301326450	1.229987138	-0.703444161
C	3.562600315	1.198839223	1.217482843
C	-3.562600315	-1.198839223	-1.217482843
C	3.645393551	2.029482206	-0.087567911
C	-3.645393551	-2.029482206	0.087567911
C	3.217024163	3.497574213	0.119016527
C	-3.217024163	-3.497574213	-0.119016527
C	-1.708521270	-3.768517266	-0.278592548
C	1.708521270	3.768517266	0.278592548
C	5.532831639	-0.375096844	1.382621474
C	-5.532831639	0.375096844	-1.382621474
C	6.485144605	0.286115653	0.387563722
C	-6.485144605	-0.286115653	-0.387563722
C	6.581180398	-0.201168824	-0.943828168
C	-6.581180398	0.201168824	0.943828168
C	7.447751084	0.424143677	-1.869916832
C	-7.447751084	-0.424143677	1.869916832
C	8.231847052	1.539761595	-1.476499624
C	-8.231847052	-1.539761595	1.476499624
C	8.148496059	2.020337923	-0.147177663
C	-8.148496059	-2.020337923	0.147177663
C	7.277335674	1.394458587	0.779407742
C	-7.277335674	-1.394458587	-0.779407742
C	1.153529704	-4.684826653	1.649280204
C	-1.153529704	4.684826653	-1.649280204
C	1.464424750	-3.781053755	-2.090399178
C	-1.464424750	3.781053755	2.090399178
H	4.170539906	1.683622494	2.009364967
H	-4.170539906	-1.683622494	-2.009364967
H	2.515724984	1.148250301	1.571552837
H	-2.515724984	-1.148250301	-1.571552837
H	3.003612107	1.559384715	-0.857773508
H	-3.003612107	-1.559384715	0.857773508
H	4.690066749	2.011797230	-0.451238785
H	-4.690066749	-2.011797230	0.451238785

H	3.726549239	3.961628322	0.989171792
H	-3.726549239	-3.961628322	-0.989171792
H	3.525621838	4.099909200	-0.761842601
H	-3.525621838	-4.099909200	0.761842601
H	5.710705615	-1.463619122	1.421028967
H	-5.710705615	1.463619122	-1.421028967
H	5.700054027	0.044761606	2.394825262
H	-5.700054027	-0.044761606	-2.394825262
H	5.972620822	-1.069907184	-1.249356878
H	-5.972620822	1.069907184	1.249356878
H	7.514175373	0.038947133	-2.903128138
H	-7.514175373	-0.038947133	2.903128138
H	8.904035880	2.029576623	-2.203395238
H	-8.904035880	-2.029576623	2.203395238
H	8.757581820	2.885825022	0.169333250
H	-8.757581820	-2.885825022	-0.169333250
H	7.214402247	1.774086813	1.815704055
H	-7.214402247	-1.774086813	-1.815704055
H	0.150326207	-5.138135035	1.776399480
H	-0.150326207	5.138135035	-1.776399480
H	1.439489593	-4.110885996	2.553853526
H	-1.439489593	4.110885996	-2.553853526
H	1.904926380	-5.483264984	1.478975558
H	-1.904926380	5.483264984	-1.478975558
H	2.331022830	-4.464065660	-2.202385323
H	-2.331022830	4.464065660	2.202385323
H	1.683568799	-2.829391834	-2.615664617
H	-1.683568799	2.829391834	2.615664617
H	0.552843359	-4.252293445	-2.508133894
H	-0.552843359	4.252293445	2.508133894

Table S4 (cont.). Selected bond lengths and angles for compound **5**

Bond lengths (Å)				
Sn1-S1	2.513	O2-C5	1.246	
Sn1-S2	2.881	C2-C3	1.549	
Sn1-O1	2.116	C3-C4	1.543	
Sn1-O2	2.907	C4-C5	1.541	
Sn1-C14	2.132	C6-C7	1.528	
Sn1-C13	2.131	C7-C8	1.421	
S1-C1	1.773	C7-C12	1.418	
S2-C1	1.732	C8-C9	1.414	
N1-C1	1.356	C9-C10	1.419	
N1-C2	1.489	C10-C11	1.416	
N1-C6	1.491	C11-C12	1.417	
O1-C5	1.321			
Angles (°)				
S1-Sn1-S2	67.4	C1-N1-C6	121.4	
S1-Sn1-O1	83.5	C2-N1-C6	116.0	
S1-Sn1-C14	114.7	N1-C2-C3	113.3	
S1-Sn1-C13	111.7	N1-C6-C7	114.4	
Sn1-S1-C1	92.6	O1-C5-O2	122.7	
S2-Sn1-O1	150.7	O1-C5-C4	116.1	
S2-Sn1-C14	89.0	C3-C2-C4	112.5	
S2-Sn1-C13	91.6	C3-C4-C5	116.9	
Sn1-S2-C1	81.7	C6-C7-C8	120.3	
O1-Sn1-C14	100.6	C6-C7-C12	120.4	
O1-Sn1-C13	102.8	C8-C7-C12	119.3	
Sn1-O1-C5	111.0	C7-C8-C9	120.2	
C14-Sn1-C13	129.8	C7-C12-C11	120.5	
S1-C1-S2	118.2	C8-C9-C10	120.3	
S1-C1-C3	118.6	C9-C10-C11	119.6	
S2-C1-N1	123.2	C10-C11-C12	120.0	
C1-N1C2	122.6			

Table S2. Calculated and experimental vibrational frequencies for $[Me_2Sn(\mathbf{L3}\text{-dtc})]_3$ (**5**).

Vibration	B3LYP/ SKBCJ(d,p)	IR data
ν_{as}(OCO)	1687	1623
ν(N-CSS)	1480	1496
ν_s(OCO)	1374	1360
ν_s(N-C_{alkyl}) + ν_s(SCS)	1227	1224
ν_{as}(N-C_{alkyl}) + ν_{as}(SCS)	1141	1137
ν_{as}(SCS)	982	981
δ(Sn-C-H)	802	777
ν(Sn-O)	670	--[a]
ν_s(SCS)	649	--[a]
ν_s(Sn-C)	507	--[a]
ν(Sn-S)	362	--[a]

[a] Could not be assigned unequivocally (several bands are present in this region).

Table S3. Selected NMR spectroscopic data for compounds **L1**·HCl, **L2**, **L3** and **1**-**7** (in $CDCl_3$, ppm).

Compound	^{1}H NMR δ(N-CH_2-spacer)	^{1}H NMR δ(N-CH_2-Ph)	^{1}H NMR δ(CH_2-COO)	^{13}C NMR δ(N-CH_2-spacer)	^{13}C NMR δ(N-CH_2-Ph)	^{13}C NMR δ(CH_2-COO)	^{13}C NMR δ(COO)	^{13}C NMR δ(CSS)	^{119}Sn NMR
L1·HCl[a]	3.88	4.29	3.88	46.9	51.1	46.9	169.2	--	--
1	4.20	5.03	4.20	55.7	60.0	55.7	171.2	200.5	-216.5
2	4.23	5.07	4.23	55.1	59.2	55.1	170.8	200.8	-222.6
L2[a]	3.12	4.14	2.48	43.9	50.8	32.5	177.8	--	--
3	3.91	5.05	2.68	51.2	58.9	33.4	176.5	199.3	-221.1
4	3.92	5.08	2.70	51.2	58.8	33.2	176.3	199.8	-230.8
L3[b]	3.06	4.14	2.35	49.3	52.1	37.2	180.9	--	--
5	3.77	5.02	2.30	54.4	57.6	32.1	178.0	199.6	-223.7
6	3.78	5.05	2.28	54.5	57.5	32.2	178.1	200.7	-230.4
7	3.81	4.96	2.31	54.6	57.6	31.8	178.5	198.2	-370.3

[a] in D_2O; [b] in CD_3OD

Table S4. Atomic coordinates and selected geometric parameters for the calculated molecular structure of compound **1** (B3LYP/SBKJC(d,p)).

C	-6.222635256	5.590306652	0.982385294
C	-1.730029947	-8.184113536	0.982385294
C	7.952665203	2.593806885	0.982385294
C	-7.011130400	6.169673417	2.009049775
C	-1.837528712	-9.156653744	2.009049775
C	8.848659113	2.986980327	2.009049775
C	-7.894437343	5.363072185	2.766977874
C	-0.697338083	-9.518319381	2.766977874
C	8.591775427	4.155247195	2.766977874
C	-7.989165329	3.973869448	2.492208083
C	0.553110771	-8.905754854	2.492208083
C	7.436054558	4.931885406	2.492208083
C	-7.205716184	3.396216179	1.465808012
C	0.661648604	-7.938441357	1.465808012
C	6.544067580	4.542225178	1.465808012
C	-6.313454837	4.201746701	0.704908894
C	-0.482091965	-7.568485624	0.704908894
C	6.795546801	3.366738924	0.704908894
C	-5.461512195	3.578623223	-0.397527575
C	-0.368422525	-6.519119915	-0.397527575
C	5.829934719	2.940496692	-0.397527575
N	-4.444300889	2.629772723	0.154407095
N	-0.055299540	-5.163763833	0.154407095
N	4.499600429	2.533991110	0.154407095
C	-3.394071455	3.243428236	0.996864678
C	-1.111855520	-4.561066221	0.996864678
C	4.505926975	1.317637985	0.996864678
C	-2.276720154	3.916192114	0.147128628
C	-2.253161780	-3.929793547	0.147128628
C	4.529881933	0.013601434	0.147128628
O	-2.553352864	4.744092595	-0.739611829
O	-2.831828274	-4.583314742	-0.739611829
O	5.385181137	-0.160777853	-0.739611829
O	-1.062553089	3.546628280	0.476789754
O	-2.540193644	-2.693512108	0.476789754
O	3.602746733	-0.853116173	0.476789754
C	-4.445843843	1.310598298	-0.140008147
C	1.087910501	-4.505512858	-0.140008147
C	3.357933342	3.194914561	-0.140008147
S	-3.190562648	0.270645548	0.559005492
S	1.360895403	-2.898431079	0.559005492
S	1.829667244	2.627785531	0.559005492
S	-5.628357750	0.564713653	-1.167947937
S	2.325122506	-5.156657619	-1.167947937
S	3.303235244	4.591943966	-1.167947937
H	-5.529607757	6.218879696	0.394814042
H	-2.620903922	-7.898220638	0.394814042

H	8.150511678	1.679340942	0.394814042
H	-6.932432541	7.252011340	2.215448261
H	-2.814209778	-9.629668361	2.215448261
H	9.746642319	2.377657021	2.215448261
H	-8.507461019	5.812392290	3.568507928
H	-0.779948870	-10.273873509	3.568507928
H	9.287409889	4.461481219	3.568507928
H	-8.680790565	3.340497564	3.076089906
H	1.447439530	-9.188033936	3.076089906
H	7.233351035	5.847536372	3.076089906
H	-7.285709945	2.315713167	1.250585879
H	1.637388543	-7.467466481	1.250585879
H	5.648321403	5.151753314	1.250585879
H	-4.906386841	4.358201315	-0.950491881
H	-1.321119633	-6.428156303	-0.950491881
H	6.227506474	2.069954987	-0.950491881
H	-6.084311933	3.003430656	-1.103359257
H	0.441108719	-6.770884026	-1.103359257
H	5.643203213	3.767453370	-1.103359257
H	-2.953421154	2.490243981	1.669234353
H	-0.679903972	-3.802859738	1.669234353
H	3.633325127	1.312615757	1.669234353
H	-3.875333086	4.033351656	1.606039584
H	-1.555318454	-5.372812729	1.606039584
H	5.430651540	1.339461073	1.606039584
Sn	-4.092001799	-1.735071071	-0.635423337
Sn	3.548616525	-2.676241975	-0.635423337
Sn	0.543385274	4.411313046	-0.635423337
C	0.067842957	3.893480607	-2.646905633
C	-3.405774594	-1.887986579	-2.646905633
C	3.337931637	-2.005494028	-2.646905633
H	0.444983476	4.685662695	-3.326268582
H	-4.280394666	-1.957464353	-3.326268582
H	3.835411190	-2.728198342	-3.326268582
H	0.560483060	2.934289987	-2.903955756
H	-2.821411201	-0.981752425	-2.903955756
H	2.260928141	-1.952537562	-2.903955756
H	-1.032060497	3.806627458	-2.745676122
H	-2.780605833	-2.797104337	-2.745676122
H	3.812666329	-1.009523120	-2.745676122
C	0.468455503	6.370231306	0.202689653
C	-5.751009890	-2.779421287	0.202689653
C	5.282554387	-3.590810019	0.202689653
H	0.979628143	7.085793820	-0.473542333
H	-6.626291525	-2.694514052	-0.473542333
H	5.646663382	-4.391279768	-0.473542333
H	0.982586427	6.373395520	1.185614772
H	-6.010815642	-2.335752953	1.185614772
H	5.028229215	-4.037642567	1.185614772
H	-0.593833780	6.662436443	0.329406065
H	-5.472922321	-3.845493361	0.329406065

H 6.066756101 -2.816943082 0.329406065

Table S4 (cont.). Selected bond lengths and angles for compound **1**

Bond lengths (Å)				
C11-C12	1.418	C3-O2	1.244	
C7-C12	1.419	C3-O1	1.311	
C10-C11	1.416	C1-S1	1.774	
C9-C10	1.419	C1-S2	1.735	
C9-C8	1.415	Sn1-S1	2.502	
C7-C8	1.423	Sn1-S2	2.817	
C6-C7	1.526	Sn1-C13	2.132	
N1-C6	1.497	Sn1-C14	2.131	
N1-C1	1.352	Sn1-O2	3.116	
C2-C3	1.557			
Angles (°)				
C7-C11-C12	120.4	C2-C3-O2	121.1	
C10-C11-C12	120.1	C2-C3-O1	113.9	
C8-C7-C12	119.3	O2-C3-O1	124.9	
C12-C7-C6	120.3	C3-Sn1-S1	149.4	
C11-C10-C9	119.7	S1-C1-S2	117.6	
C10-C9-C8	120.2	C1-S1-Sn1	91.5	
C9-C8-C7	120.3	C1-S2-Sn1	82.4	
C8-C7-C6	120.3	S1-Sn1-S2	68.4	
C7-C6-N1	118.8	S1-Sn1-C14	113.1	
C6-N1-C1	122.5	S1-Sn1-C13	119.0	
N1-C2-C3	112.2	S2-Sn1-C14	93.2	
C2-N1-C1	122.0	S2-Sn1-C13	92.9	
N1-C1-S1	119.1	C14-Sn1-C13	125.9	
N1-C1-S2	123.3			