Electronic Supplementary Information

Phosphate-induced fluorescence of a tetraphenylethene-substituted tripodal tris(urea) receptor

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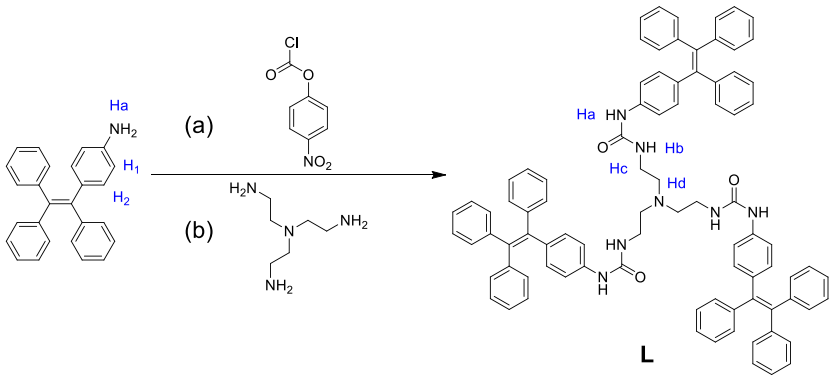

Scheme 1. Synthesis of ligands **L**. (a) THF, reflux; (b) triethylamine, THF, reflux.

Table S1. Crystal data and structure refinement of ligand **L** and complexes **1** and **2**.

Compound	**L**	**1**·CH_2Cl_2	**2**·DMF
Empirical formula	$C_{87}H_{75}N_7O_3$	$C_{100}H_{105}Cl_3N_8O_4$	$C_{110}H_{132}N_{10}O_9P$
*F*w	1266.54	1589.27	1769.23
Crystal color	colorless	yellow	yellow
T /K	298	100	100
Crystal system	Triclinic	Monoclinic	Triclinic
Space group	*P*-1	*P*2(1)/*n*	*P*-1
a /Å	13.720(4)	23.826(5)	17.001(3)
b /Å	15.939(5)	14.975(3)	17.176(3)
c /Å	19.972(6)	26.604(5)	18.944(4)
α /°	70.578(7)	90	82.554(3)
β /°	78.928(7)	111.883(2)	84.382(3)
γ /°	70.749(7)	90	84.457(3)
V /Å^3	3872(2)	8809(3)	5439.0(19)
Z	2	4	2
D_{calc} /g cm^{-3}	1.086	1.198	1.080
F (000)	1340	3376.0	1898.0
μ /mm^{-1}	0.066	0.161	0.083
Crystal size (mm^3)	0.25×0.20×0.20	0.35×0.31×0.28	0.35×0.31×0.28
θ range (°)	1.41 to 25.02	1.59 to 25.27	2.35 to 25.00
Reflections collected	21516	56116	33817
Independent reflections	13404	15622	18331
Observed reflections [I >2σ(I)]	5258	10627	9801
R_{int}	0.0564	0.0480	0.0468
Refined parameters	851	1042	1176
Goodness of fit on F^2	1.022	1.183	1.142
$R1$ [I > 2σ(I)]	0.0829	0.0875	0.1249
$wR2$ (all data)	0.1891	0.2614	0.2721

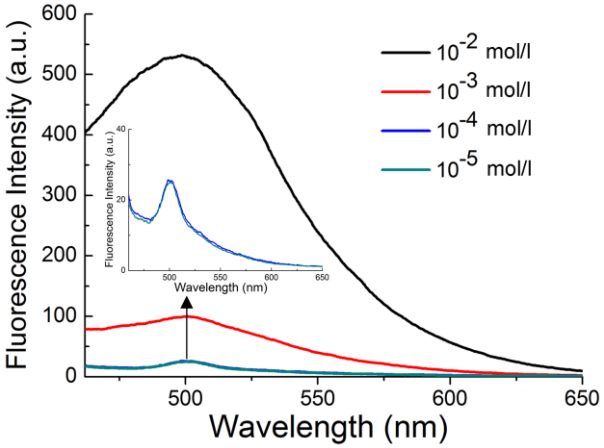

Fig. S1. Fluorescence emission spectra (λ_{ex} = 435 nm) of **L** in different concentrations (in DMSO).

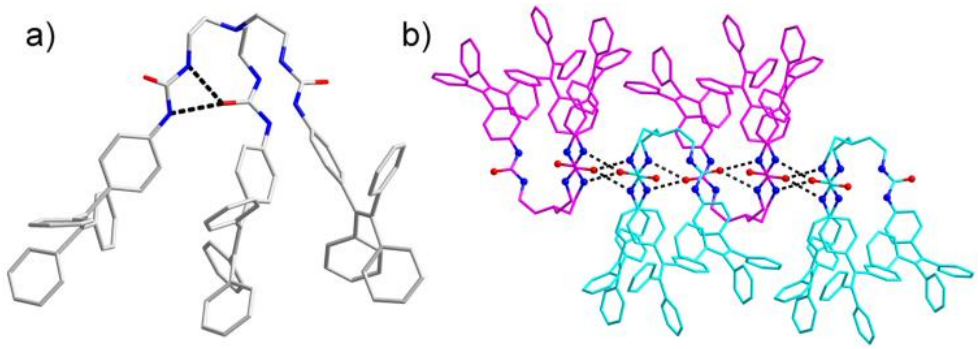

Fig. S2. a) Crystal structure of **L** showing the intramolecular N−H···O hydrogen bonds. b) 1D urea-tape formed by the hydrogen bonding of the urea moieties. The N (blue) and O (red) atoms of urea are shown in the ball-and-stick model.

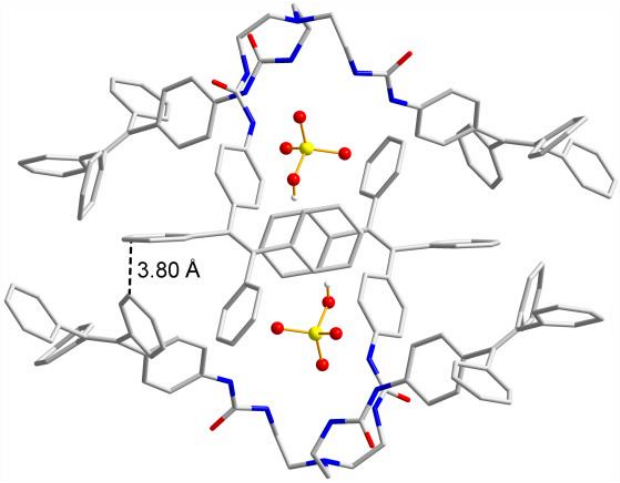

Fig. S3. Intermolecular interactions in complex $(TEA)_2[HPO_4 \subset \mathbf{L}]\cdot DMF$ (**2**).

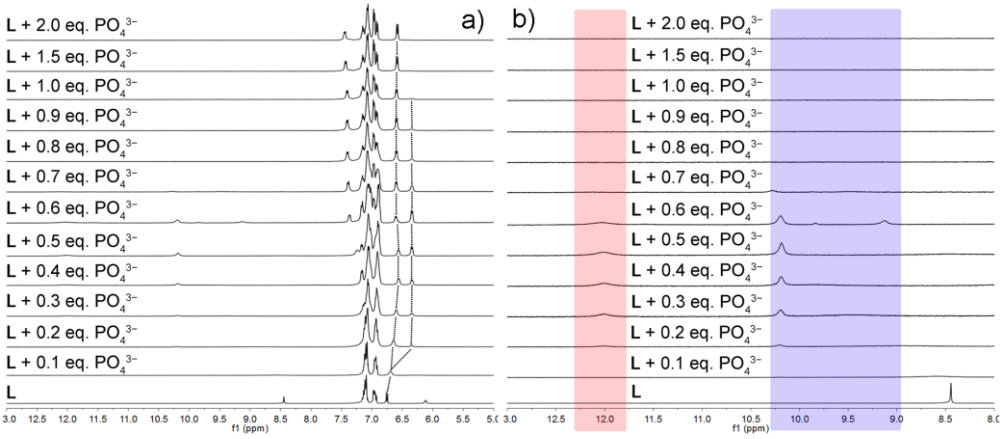

Fig. S4. a) ^{1}H NMR titration of **L** (5 mM) with 0–2.0 equiv of PO_4^{3-} (as TBA^+ salt) in DMSO-d_6. b) Partial ^{1}H NMR spectra of **L** (5 mM) with 0.1–2.0 equiv. of PO_4^{3-} in DMSO-d_6. The red and blue areas highlight the signals of NHa and NHb.

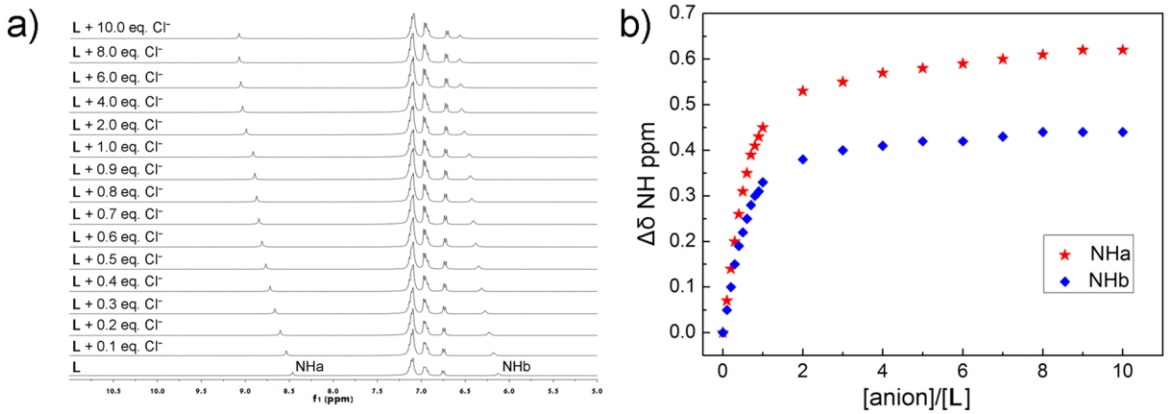

Fig. S5. a) ^{1}H NMR titration of **L** (5 mM) with TEACl in DMSO-d_6. b) ^{1}H NMR titration curves showing the net changes in the chemical shifts of NHa and NHb.

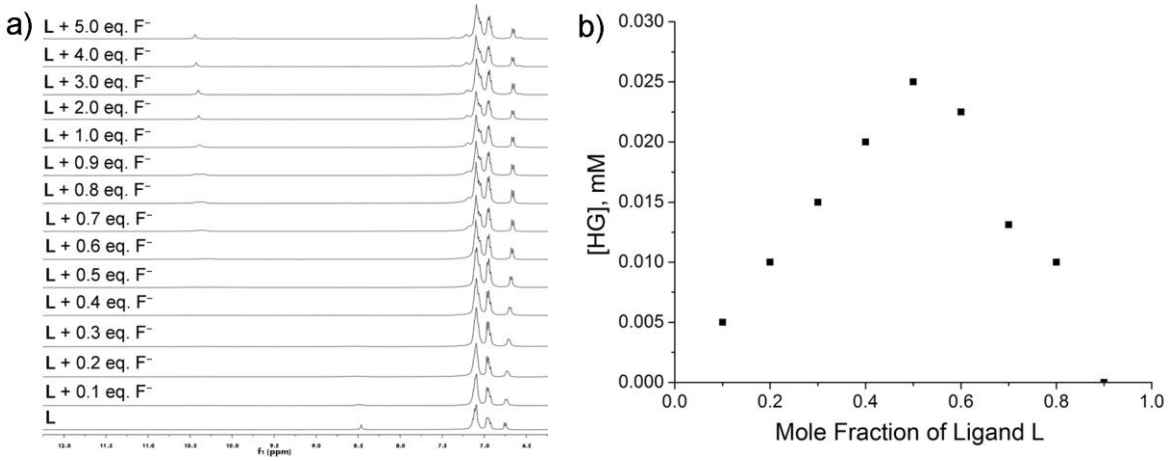

Fig. S6. a) ^{1}H NMR titration of **L** (5 mM) with F^{-} (as TBA^{+} salt) in DMSO-d_6. b) Job's plot of **L** with F^{-}.

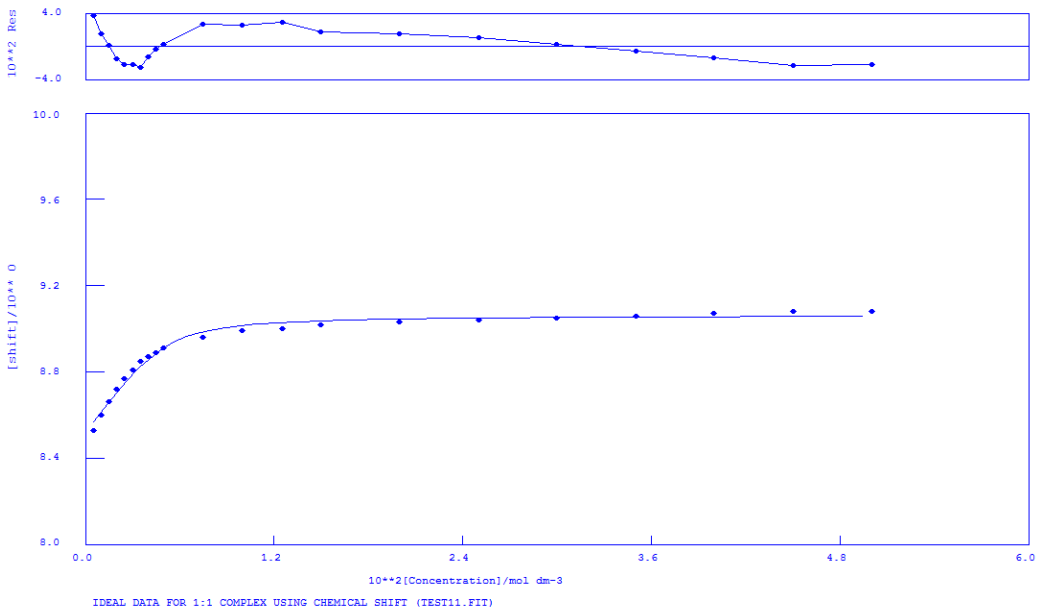

Fig. S7. ^{1}H NMR titration of **L** with Cl^{-} in DMSO-d_6.

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 08:39:52 on 01/13/2015

IDEAL DATA FOR 1:1 COMPLEX USING CHEMICAL SHIFT (TEST11.FIT)
Reaction: M + L = ML
FILE: TEST11.FIT
IDEAL DATA: K1 = 1000; DELTA M = 8.46; DELTA ML = 9.08
File prepared by M. J. Hynes, October 22 2000

NO.	A	PARAMETER	DELTA	ERROR	CONDITION	DESCRIPTION
1	1	1.86654E+03	2.000E-01	1.094E+02	1.047E+00	K1
2	1	8.51791E+00	2.000E-01	1.196E-02	1.211E+00	SHIFT M
3	1	9.06266E+00	5.000E-02	6.338E-03	1.161E+00	SHIFT ML

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RFACTOR = 0.2153 PERCENT

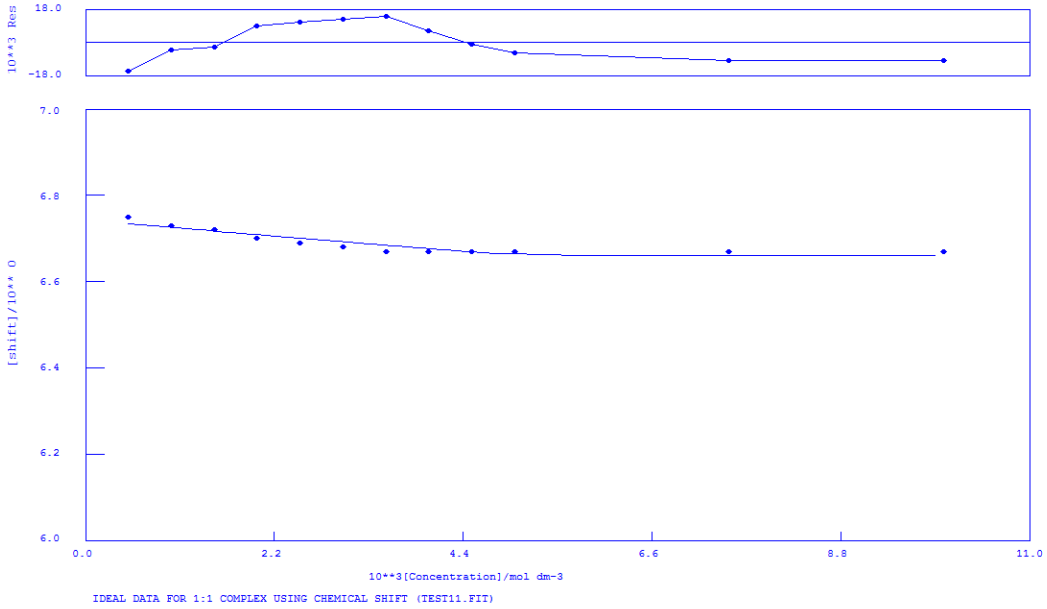

Fig. S8. ^{1}H NMR titration of **L** with F^{-} in DMSO-d_6.

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 08:48:22 on 01/13/2015

IDEAL DATA FOR 1:1 COMPLEX USING CHEMICAL SHIFT (TEST11.FIT)
Reaction: M + L = ML
FILE: TEST11.FIT
IDEAL DATA: K1 = 52450; DELTA M = 6.76; DELTA ML = 6.67
File prepared by M. J. Hynes, October 22 2000

NO.	A	PARAMETER	DELTA	ERROR	CONDITION	DESCRIPTION
1	1	5.19870E+04	2.000E-01	3.103E+03	1.011E+00	K1
2	1	6.74261E+00	2.000E-01	7.235E-03	1.241E+00	SHIFT M

3 1 6.65872E+00 5.000E-02 5.175E-03 1.234E+00 SHIFT ML

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RESIDUALS SQUARED = 1.10E-03
RFACTOR = 0.1429 PERCENT

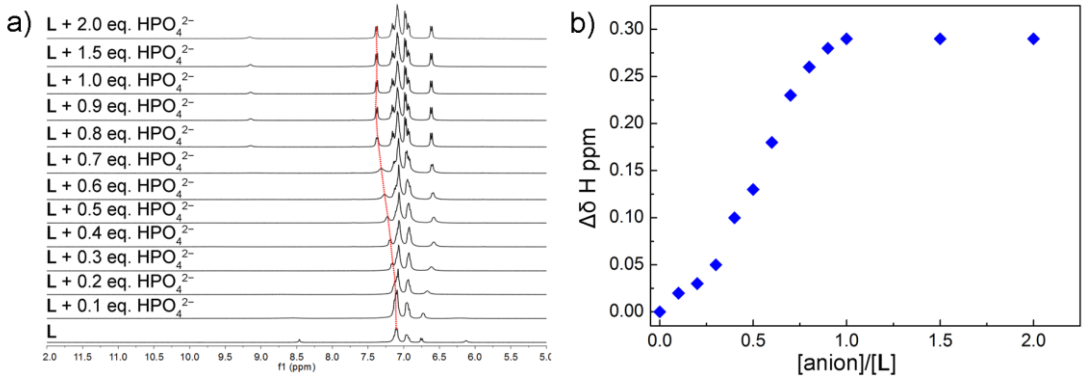

Fig. S9. a) ^{1}H NMR titration of **L** (5 mM) with $(TBA)_2HPO_4$ in DMSO-d_6. b) ^{1}H NMR titration curves showing the net changes in the chemical shifts of one of the aromatic H signal (red dotted line in a).

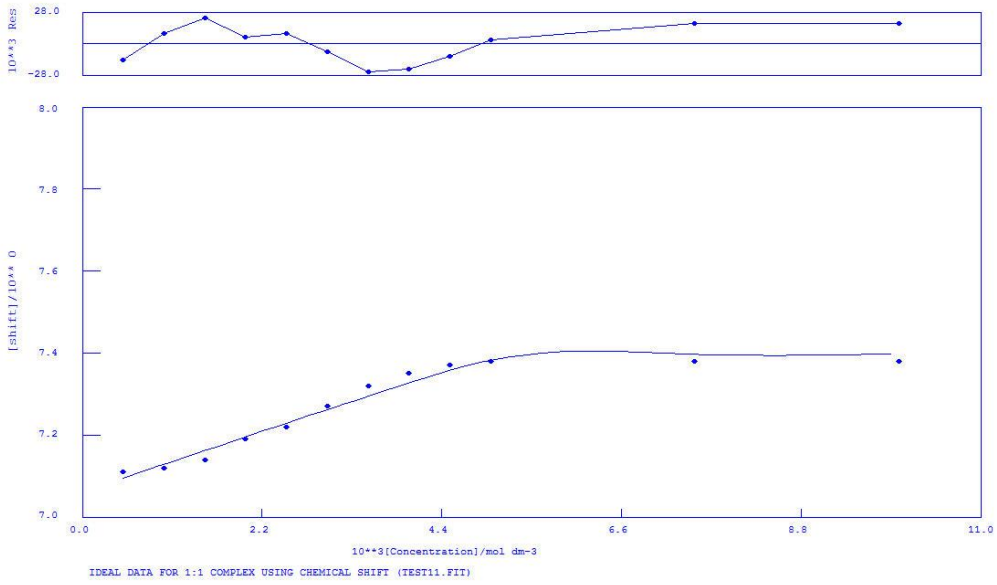

Fig. S10. ^{1}H NMR titration of **L** with HPO_4^{2-} in DMSO-d_6.

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 06:55:07 on 01/30/2016

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Reaction: M + L = ML
FILE: TEST11.FIT
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File prepared by M. J. Hynes, October 22 2000

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION
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2 1 7.06199E+00 2.000E-01 1.230E-02 1.363E+00 SHIFT M
3 1 7.39789E+00 5.000E-02 8.626E-03 1.329E+00 SHIFT ML

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RFACTOR = 0.2126 PERCENT

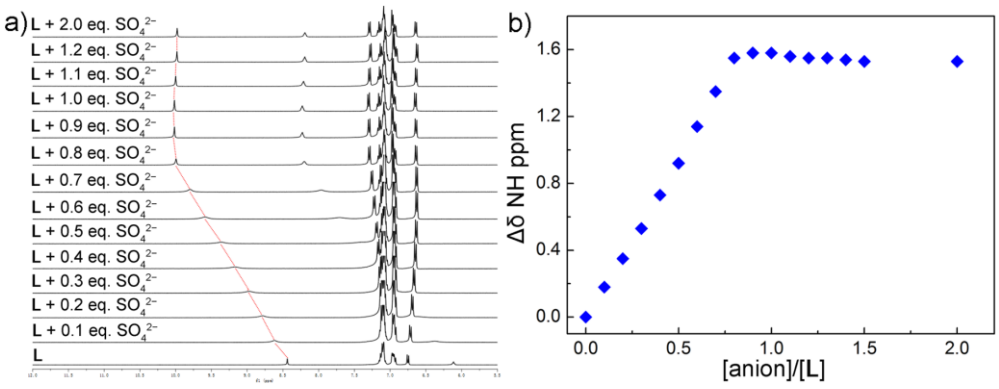

Fig. S11. a) ^{1}H NMR titration of **L** (5 mM) with $(TBA)_2SO_4$ in DMSO-d_6. b) ^{1}H NMR titration curves showing the net changes in the chemical shifts of NH.

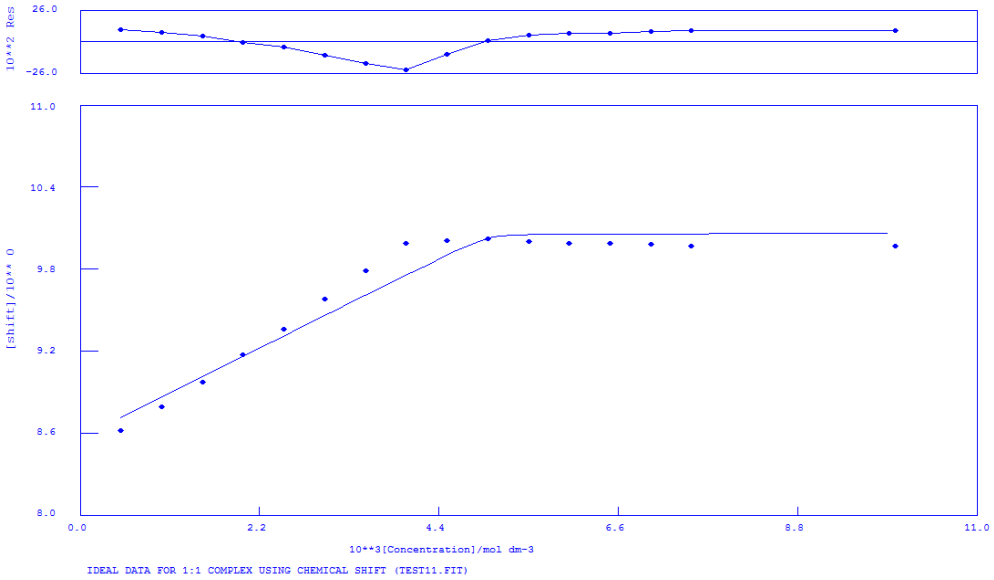

Fig. S12. ^{1}H NMR titration of **L** with SO_4^{2-} in DMSO-d_6.

Calculations by WinEQNMR Version 1.20 by Michael J. Hynes
Program run at 06:03:23 on 02/18/2016

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Reaction: M + L = ML
FILE: TEST11.FIT
IDEAL DATA: K1 = 292430; DELTA M = 8.44; DELTA ML = 9.97
File prepared by M. J. Hynes, October 22 2000

NO. A PARAMETER DELTA ERROR CONDITION DESCRIPTION

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2 1 8.56573E+00 2.000E-01 7.059E-02 1.115E+00 SHIFT M
3 1 1.00586E+01 5.000E-02 4.088E-02 1.277E+00 SHIFT ML

0RMS ERROR = 1.13E-01 MAX ERROR = 2.34E-01 AT OBS.NO. 8
RESIDUALS SQUARED = 1.66E-01
RFACTOR = 1.0552 PERCENT

DFT molecular modeling

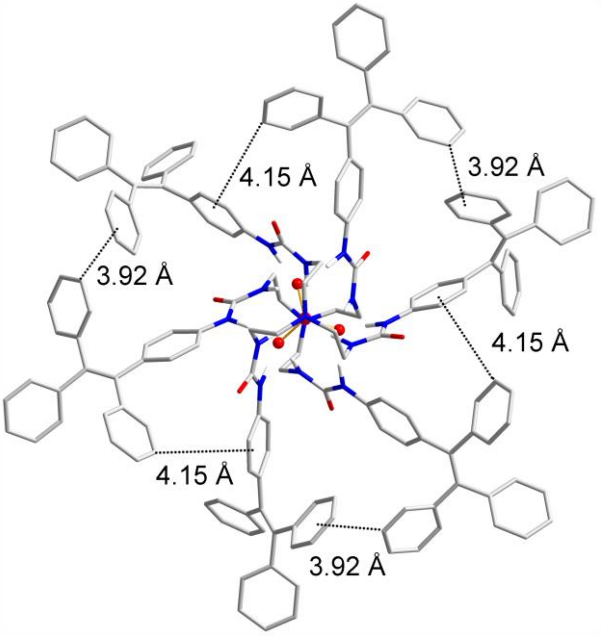

Fig. S13. C–H ··π interactions between the aryl rings of the adjacent TPE groups in complex $[PO_4 \subset \mathbf{L}_2]^{3-}$.

Cartesian coordinates (Å) for the optimized geometries of $[PO_4 \subset \mathbf{L}_2]^{3-}$

N1	0.0000	0.0000	5.1076	C176	-8.4216	0.1054	-0.4219
C2	-0.0489	-3.3729	2.9457	C177	-9.3047	-0.6866	0.2643
C3	-0.3779	-1.3823	5.4833	C178	-8.7239	0.6375	-1.7876
H4	-0.8105	-1.4300	6.5031	C179	-10.7293	-0.8544	-0.1552
H5	0.5188	-2.0088	5.4754	C180	-8.9111	-1.4675	1.4788
C6	-1.3597	-2.0094	4.4681	C181	-8.4105	1.9716	-2.1021
H7	-1.6719	-2.9871	4.8460	C182	-9.2573	-0.1831	-2.7961
H8	-2.2352	-1.3651	4.3425	C183	-11.5342	0.2543	-0.4749
N9	0.5091	-3.4421	1.6568	C184	-11.3158	-2.1344	-0.1984
H10	0.2643	-2.6907	0.9641	C185	-7.6809	-2.1517	1.5397
N11	-0.7375	-2.2096	3.1583	C186	-9.7905	-1.5783	2.5715
H12	-0.5133	-1.3443	2.5991	H187	-7.9577	2.5937	-1.3398
C13	1.3860	0.3639	5.4833	C188	-8.6557	2.4798	-3.3774
H14	1.6436	0.0131	6.5031	C189	-9.4908	0.3227	-4.0743

H15	1.4803	1.4537	5.4754	H190	-9.4737	-1.2192	-2.5706
C16	2.4201	-0.1728	4.4681	H191	-11.0971	1.2440	-0.4378
H17	3.4229	0.0456	4.8460	C192	-12.8691	0.0879	-0.8431
H18	2.2998	-1.2532	4.3425	H193	-10.7120	-2.9946	0.0655
C19	2.9455	1.6441	2.9457	C194	-12.6493	-2.3001	-0.5709
N20	2.7264	2.1619	1.6568	H195	-6.9843	-2.0638	0.7165
H21	2.1981	1.5743	0.9641	C196	-7.3431	-2.9106	2.6591
N22	2.2823	0.4661	3.1583	C197	-9.4477	-2.3354	3.6931
H23	1.4209	0.2276	2.5991	H198	-10.7432	-1.0634	2.5335
C24	-1.0081	1.0184	5.4833	H199	-8.4065	3.5110	-3.6018
H25	-0.8331	1.4169	6.5031	C200	-9.1980	1.6572	-4.3685
H26	-1.9991	0.5551	5.4754	H201	-9.8864	-0.3292	-4.8455
C27	-1.0604	2.1823	4.4681	H202	-13.4703	0.9579	-1.0854
H28	-1.7510	2.9415	4.8460	H203	-13.0763	-3.2969	-0.6074
H29	-0.0646	2.6183	4.3425	H204	-6.3859	-3.4190	2.6865
C30	-2.8966	1.7288	2.9457	C205	-8.2234	-3.0049	3.7422
N31	-3.2355	1.2802	1.6568	H206	-10.1354	-2.3977	4.5302
H32	-2.4624	1.1164	0.9641	H207	-9.3712	2.0469	-5.3657
N33	-1.5448	1.7435	3.1583	H208	-7.9531	-3.5906	4.6137
H34	-0.9076	1.1167	2.5991	C209	-3.0178	-3.4423	-1.1136
N35	0.0000	0.0000	-4.6674	C210	-2.6791	-3.9678	0.1572
C36	-2.3115	0.5612	-3.8510	C211	-3.8739	-4.2122	-1.9392
H37	-1.9784	1.5695	-3.5992	H212	-2.0494	-3.3845	0.8165
H38	-3.3490	0.6000	-4.2059	C213	-3.1308	-5.2124	0.5574
C39	-1.4380	-0.0328	-4.9806	H214	-4.1212	-3.8064	-2.9074
H40	-1.7588	-1.0720	-5.0972	C215	-4.3249	-5.4538	-1.5230
H41	-1.6710	0.4969	-5.9247	C216	-3.9600	-6.0010	-0.2740
C42	-2.7826	-1.4960	-2.6342	H217	-2.8295	-5.5924	1.5262
N43	-2.2360	-0.2438	-2.6281	H218	-4.9512	-6.0361	-2.1877
H44	-1.7983	0.1629	-1.7753	C219	-4.3324	-7.3820	0.1090
N45	-2.4735	-2.2245	-1.4757	C220	-5.5420	-7.9598	-0.1942
H46	-1.6400	-1.8950	-0.9130	C221	-3.2709	-8.1356	0.8536
C47	0.6697	-2.2825	-3.8510	C222	-5.7751	-9.4327	-0.1189
H48	-0.3700	-2.4981	-3.5992	C223	-6.7308	-7.1640	-0.6299
H49	1.1549	-3.2003	-4.2059	C224	-1.9195	-8.0052	0.4845
C50	0.7474	-1.2290	-4.9806	C225	-3.5841	-8.9116	1.9834
H51	1.8078	-0.9872	-5.0972	C226	-4.8464	-10.3505	-0.6463
H52	0.4052	-1.6956	-5.9247	C227	-6.9650	-9.9431	0.4375
C53	2.6869	-1.6618	-2.6342	C228	-7.1079	-5.9900	0.0474
N54	1.3291	-1.8145	-2.6281	C229	-7.5358	-7.6031	-1.6980
H55	0.7581	-1.6389	-1.7753	H230	-1.6649	-7.3728	-0.3562
N56	3.1632	-1.0299	-1.4757	C231	-0.9136	-8.6374	1.2154
H57	2.4611	-0.4728	-0.9130	C232	-2.5792	-9.5502	2.7087
C58	0.6906	1.2617	-4.9806	H233	-4.6182	-8.9989	2.2911

H59	-0.0489	2.0592	-5.0972	H234	-3.9331	-9.9725	-1.0873
H60	1.2659	1.1987	-5.9247	C235	-5.0877	-11.7226	-0.5981
C61	1.6418	1.7212	-3.8510	H236	-7.6975	-9.2464	0.8272
H62	2.3484	0.9286	-3.5992	C237	-7.2036	-11.3162	0.4882
H63	2.1941	2.6003	-4.2059	H238	-6.4947	-5.6353	0.8656
C64	0.0957	3.1578	-2.6342	C239	-8.2377	-5.2720	-0.3389
N65	-0.6897	3.2544	-1.4757	C240	-8.6651	-6.8813	-2.0876
H66	-0.8212	2.3678	-0.9130	H241	-7.2619	-8.5112	-2.2223
N67	0.9068	2.0583	-2.6281	H242	0.1239	-8.4847	0.9403
H68	1.0403	1.4759	-1.7753	C243	-1.2408	-9.4165	2.3280
P69	0.0000	0.0000	0.2482	H244	-2.8381	-10.1340	3.5857
O70	0.0000	0.0000	1.8710	H245	-4.3562	-12.4093	-1.0108
O71	1.4082	0.6380	-0.2842	H246	-8.1226	-11.6854	0.9319
O72	-1.2566	0.9006	-0.2842	H247	-8.4937	-4.3643	0.1954
O73	-0.1516	-1.5386	-0.2842	C248	-9.0205	-5.7120	-1.4111
O74	0.0504	-4.2830	3.8078	H249	-9.2618	-7.2278	-2.9252
O75	-3.7343	2.0978	3.8078	H250	-0.4577	-9.8918	2.9084
O76	3.6839	2.1851	3.8078	H251	-9.8917	-5.1431	-1.7175
O77	-3.4697	-1.9353	-3.5927	C252	4.4900	-0.8923	-1.1136
O78	3.4108	-2.0372	-3.5927	C253	4.7758	-0.3363	0.1572
O79	0.0588	3.9724	-3.5927	C254	5.5848	-1.2488	-1.9392
C80	3.1794	3.3851	1.1916	H255	3.9557	-0.0826	0.8165
C81	2.8637	3.7458	-0.1411	C256	6.0795	-0.1051	0.5574
C82	3.9323	4.3035	1.9639	H257	5.3571	-1.6659	-2.9074
H83	2.2926	3.0570	-0.7485	C258	6.8855	-1.0185	-1.5230
C84	3.2596	4.9639	-0.6660	C259	7.1771	-0.4289	-0.2740
H85	4.2041	4.0036	2.9631	H260	6.2579	0.3458	1.5262
C86	4.2927	5.5349	1.4372	H261	7.7030	-1.2698	-2.1877
C87	3.9607	5.9042	0.1193	C262	8.5592	-0.0610	0.1090
H88	2.9926	5.2113	-1.6873	C263	9.6643	-0.8196	-0.1942
H89	4.8388	6.2380	2.0567	C264	8.6811	1.2351	0.8536
C90	4.3021	7.2407	-0.4219	C265	11.0566	-0.2850	-0.1189
C91	4.0577	8.4014	0.2643	C266	9.5696	-2.2470	-0.6299
C92	4.9140	7.2364	-1.7876	C267	7.8925	2.3403	0.4845
C93	4.6247	9.7191	-0.1552	C268	9.5097	1.3519	1.9834
C94	3.1847	8.4510	1.4788	C269	11.3869	0.9782	-0.6463
C95	5.9127	6.2979	-2.1021	C270	12.0935	-1.0603	0.4375
C96	4.4701	8.1086	-2.7961	C271	8.7415	-3.1606	0.0474
C97	5.9874	9.8618	-0.4749	C272	10.3523	-2.7246	-1.6980
C98	3.8095	10.8670	-0.1984	H273	7.2174	2.2446	-0.3562
C99	1.9771	7.7277	1.5397	C274	7.9371	3.5275	1.2154
C100	3.5284	9.2679	2.5715	C275	9.5603	2.5415	2.7087
H101	6.2251	5.5947	-1.3398	H276	10.1024	0.4999	2.2911
C102	6.4754	6.2561	-3.3774	H277	10.6030	1.5801	-1.0873

C103	5.0249	8.0579	-4.0743	C278	12.6959	1.4552	-0.5981
H104	3.6810	8.8141	-2.5706	H279	11.8564	-2.0430	0.8272
H105	6.6259	8.9883	-0.4378	C280	13.4019	-0.5804	0.4882
C106	6.5107	11.1010	-0.8431	H281	8.1276	-2.8069	0.8656
H107	2.7626	10.7741	0.0655	C282	8.6845	-4.4981	-0.3389
C108	4.3327	12.1047	-0.5709	C283	10.2919	-4.0635	-2.0876
H109	1.7049	7.0805	0.7165	H284	11.0019	-2.0334	-2.2223
C110	1.1508	7.8146	2.6591	H285	7.2860	4.3497	0.9403
C111	2.7013	9.3496	3.6931	C286	8.7753	3.6337	2.3280
H112	4.4507	9.8356	2.5335	H287	10.1954	2.6091	3.5857
H113	7.2439	5.5248	-3.6018	H288	12.9248	2.4320	-1.0108
C114	6.0342	7.1370	-4.3685	H289	14.1812	-1.1917	0.9319
H115	4.6581	8.7265	-4.8455	H290	8.0265	-5.1737	0.1954
H116	7.5647	11.1867	-1.0854	C291	9.4570	-4.9560	-1.4111
H117	3.6830	12.9729	-0.6074	H292	10.8904	-4.4071	-2.9252
H118	0.2320	7.2399	2.6865	H293	8.7954	4.5495	2.9084
C119	1.5094	8.6242	3.7422	H294	9.3999	-5.9949	-1.7175
H120	2.9912	9.9764	4.5302	C295	1.3419	-4.4460	1.1916
H121	6.4583	7.0923	-5.3657	C296	1.8121	-4.3530	-0.1411
H122	0.8670	8.6829	4.6137	C297	1.7608	-5.5572	1.9639
C123	-1.4722	4.3346	-1.1136	H298	1.5012	-3.5140	-0.7485
C124	-2.0967	4.3041	0.1572	C299	2.6690	-5.3048	-0.6660
C125	-1.7109	5.4610	-1.9392	H300	1.3652	-5.6426	2.9631
H126	-1.9063	3.4671	0.8165	C301	2.6470	-6.4851	1.4372
C127	-2.9487	5.3176	0.5574	C302	3.1328	-6.3822	0.1193
H128	-1.2358	5.4723	-2.9074	H303	3.0168	-5.1974	-1.6873
C129	-2.5607	6.4723	-1.5230	H304	2.9829	-7.3095	2.0567
C130	-3.2171	6.4300	-0.2740	C305	4.1196	-7.3460	-0.4219
H131	-3.4284	5.2466	1.5262	C306	5.2470	-7.7148	0.2643
H132	-2.7518	7.3059	-2.1877	C307	3.8099	-7.8739	-1.7876
C133	-4.2268	7.4430	0.1090	C308	6.1046	-8.8647	-0.1552
C134	-4.1224	8.7794	-0.1942	C309	5.7264	-6.9835	1.4788
C135	-5.4101	6.9005	0.8536	C310	2.4978	-8.2695	-2.1021
C136	-5.2814	9.7178	-0.1189	C311	4.7872	-7.9255	-2.7961
C137	-2.8388	9.4111	-0.6299	C312	5.5469	-10.1161	-0.4749
C138	-5.9730	5.6649	0.4845	C313	7.5063	-8.7326	-0.1984
C139	-5.9256	7.5597	1.9834	C314	5.7039	-5.5761	1.5397
C140	-6.5406	9.3723	-0.6463	C315	6.2621	-7.6896	2.5715
C141	-5.1285	11.0034	0.4375	H316	1.7327	-8.1884	-1.3398
C142	-1.6336	9.1506	0.0474	C317	2.1802	-8.7360	-3.3774
C143	-2.8166	10.3277	-1.6980	C318	4.4659	-8.3806	-4.0743
H144	-5.5526	5.1282	-0.3562	H319	5.7927	-7.5949	-2.5706
C145	-7.0234	5.1099	1.2154	H320	4.4712	-10.2324	-0.4378
C146	-6.9812	7.0087	2.7087	C321	6.3584	-11.1889	-0.8431

H147	-5.4841	8.4989	2.2911	H322	7.9493	-7.7796	0.0655
H148	-6.6699	8.3924	-1.0873	C323	8.3166	-9.8045	-0.5709
C149	-7.6082	10.2674	-0.5981	H324	5.2795	-5.0167	0.7165
H150	-4.1589	11.2895	0.8272	C325	6.1922	-4.9040	2.6591
C151	-6.1983	11.8966	0.4882	C326	6.7464	-7.0142	3.6931
H152	-1.6329	8.4422	0.8656	H327	6.2925	-8.7722	2.5335
C153	-0.4468	9.7700	-0.3389	H328	1.1626	-9.0358	-3.6018
C154	-1.6269	10.9448	-2.0876	C329	3.1638	-8.7943	-4.3685
H155	-3.7400	10.5446	-2.2223	H330	5.2283	-8.3973	-4.8455
H156	-7.4099	4.1351	0.9403	H331	5.9056	-12.1446	-1.0854
C157	-7.5345	5.7828	2.3280	H332	9.3934	-9.6760	-0.6074
H158	-7.3573	7.5249	3.5857	H333	6.1539	-3.8209	2.6865
H159	-8.5686	9.9772	-1.0108	C334	6.7141	-5.6192	3.7422
H160	-6.0586	12.8771	0.9319	H335	7.1442	-7.5786	4.5302
H161	0.4673	9.5379	0.1954	H336	2.9129	-9.1392	-5.3657
C162	-0.4365	10.6680	-1.4111	H337	7.0861	-5.0923	4.6137
H163	-1.6285	11.6349	-2.9252	C338	-6.2656	-12.2150	-0.0281
H164	-8.3377	5.3423	2.9084	C339	-13.4338	-1.1895	-0.8963
H165	0.4918	11.1380	-1.7175	C340	13.7113	0.6813	-0.0281
C166	-4.5213	1.0609	1.1916	C341	-7.4457	11.5337	-0.0281
C167	-4.6758	0.6072	-0.1411	C342	5.6868	12.2288	-0.8963
C168	-5.6931	1.2537	1.9639	C343	7.7470	-11.0393	-0.8963
H169	-3.7938	0.4570	-0.7485	H344	-6.4519	-13.2831	0.0082
C170	-5.9286	0.3410	-0.6660	H345	8.3773	-11.8743	-1.1829
H171	-5.5692	1.6390	2.9631	H346	14.7294	1.0541	0.0082
C172	-6.9397	0.9501	1.4372	H347	6.0948	13.1921	-1.1829
C173	-7.0935	0.4780	0.1193	H348	-8.2776	12.2290	0.0082
H174	-6.0095	-0.0140	-1.6873	H349	-14.4721	-1.3178	-1.1829
H175	-7.8216	1.0715	2.0567				