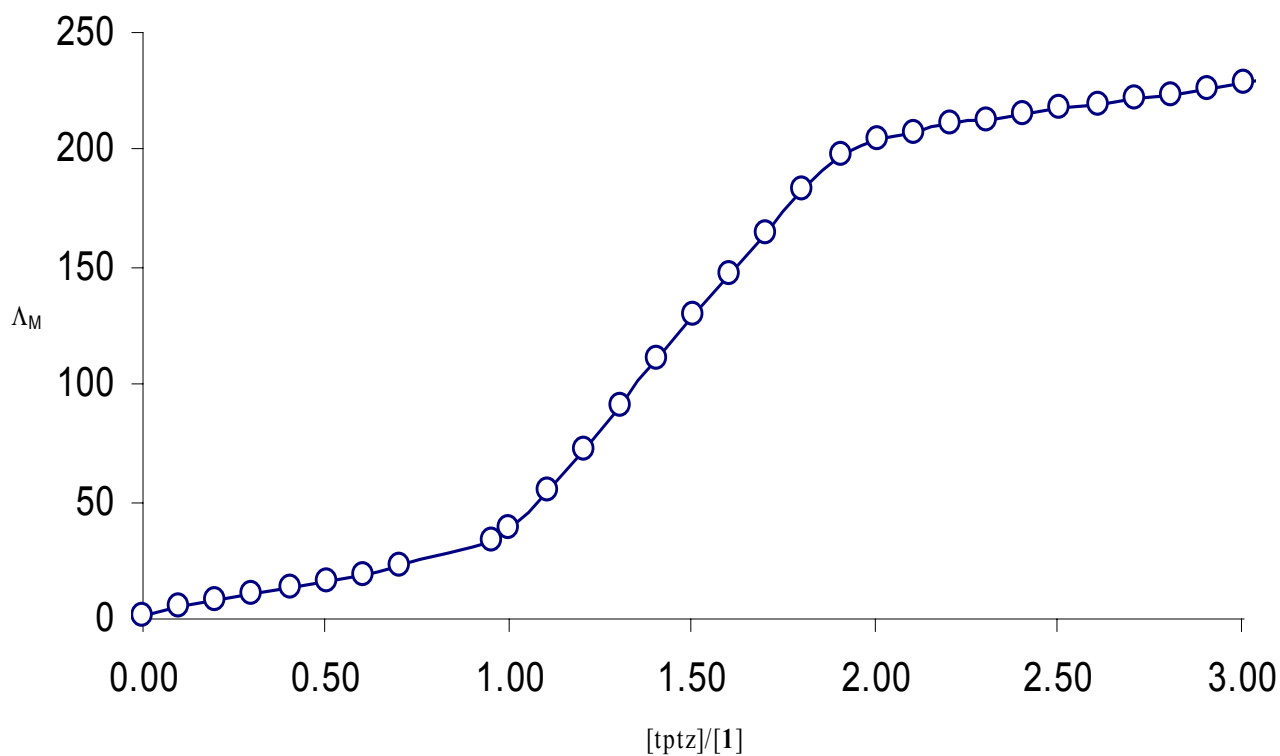
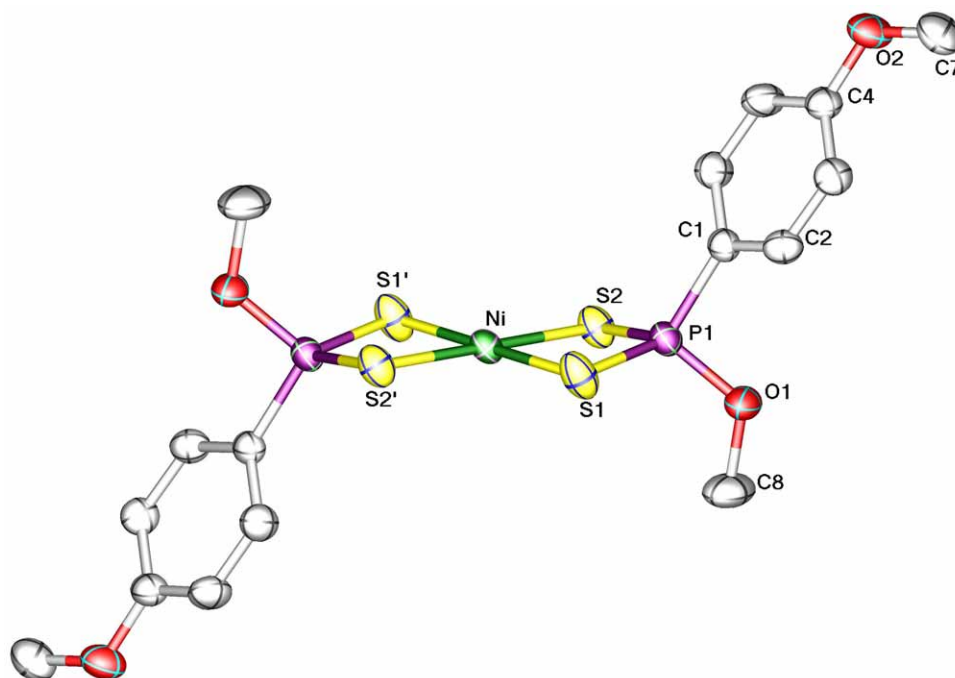


**Fig. S1** Plot of molar conductivity  $\Lambda_M$  ( $\text{S}\cdot\text{cm}^2\cdot\text{mol}^{-1}$ ) recorded during the titration of **1** ( $9.98\cdot 10^{-2}$  M) with tptz ( $1.00\cdot 10^{-1}$  M) vs. [tptz]/[**1**] molar ratio.



**Fig. S2** Molecular view of **1**. For clarity, only non-carbon atoms have been labelled and hydrogen atoms are omitted. Displacement ellipsoids are drawn at 50% probability.  $\prime$ : 1-x, 1-y, 1-z.



**Table S1** Selected hydrogen bond distances (Å) and angles (°) for compounds **3**·4H<sub>2</sub>O, **6** and **7**.

<b>Compound 3·4H<sub>2</sub>O</b>					
O6–H6D···O5	0.84(1)	1.91(1)	2.746(3)	172(3)	1-x, -y, -z
C8–H8···O1	0.95	2.34	3.206(3)	152	x, 0.5-y, 0.5+z
C29–H29···O5	0.95	2.40	3.147(3)	135	1-x, -0.5+y, 0.5-z
C31–H31···O8	0.95	2.41	3.056(4)	125	
C10–H10···O8	0.85	2.49	3.159	137	1-x, -y, -z
O5–H5C···N12	0.84(1)	1.98(1)	2.799(3)	165(3)	x, 0.5-y, -0.5+z
O6–H6C···N6	0.84(1)	2.06(1)	2.875(3)	164(3)	
C44–H44A···N2	0.98	2.49	3.359(4)	147	
O7–H7C···S3	0.97(1)	2.30(1)	3.249(3)	166(3)	
O8–H8D···S4	0.96(1)	2.54(2)	3.441(3)	157(3)	
C34–H34···S1	0.95	2.78	3.707(3)	166	2-x, -0.5+y, 0.5-z
C30–H30···S4	0.95	2.78	3.532(3)	137	
C13–H13···S3	0.95	2.86	3.716(3)	150	1-x, -0.5+y, 0.5-z
C36–H36···S4	0.95	2.82	3.568(3)	137	1-x, -y, 1-z
C38–H38···S2	0.95	2.83	3.342(3)	115	
<b>Compound 5</b>					
C15–H15···N3	0.95	2.41	2.748(9)	101	
C33–H33···N9	0.95	2.41	2.752(8)	101	
C8–H8···I1	0.95	3.00	3.891(6)	157	1+x, y, z
C17–H17···I3	0.95	3.04	3.993(8)	177	-x, 1-y, -z
C29–H29···I6	0.95	2.97	3.623(7)	127	1+x, y, z
C31–H31···I4	0.95	3.01	3.729(5)	133	
C31–H31···I5	0.95	3.06	3.970(6)	161	
<b>Compound 6</b>					
C16–H16···Br1	0.95	2.89	3.739(5)	150	1-x, 1-y, -z
C17–H17···Br2	0.95	2.97	3.660	130	0.5+x, 0.5+y, z
C7–H7···Br1	0.95	3.04	3.759	135	0.5-x, 0.5+y, 0.5-z
C12–H12···Br1	0.95	3.05	3.893	149	0.5-x, 0.5-y, -z