Solution versus Solid-State Structure of Ytterbium Heterobimetallic Catalysts

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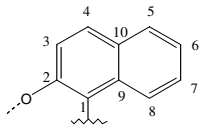
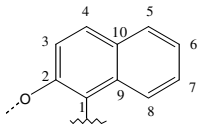
Supporting Information

Table S1. Cartesian coordinates (Å) of the solution structure of $Na_3[Yb((S)\text{-BINOL})_3]$ (**1**) obtained through the computer program PERSEUS.



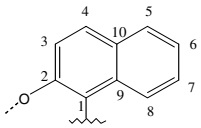
Solution Structure Coordinates			
Atom	**X coordinate**	**Y coordinate**	**Z coordinate**
BINOL 1			
O2’	1.802	-0.102	-1.261
C2’	2.122	-1.345	-1.590
C3’	1.915	-1.688	-2.955
C4’	2.208	-2.938	-3.391
C10’	2.679	-3.931	-2.541
C5’	2.941	-5.253	-3.026
C6’	3.403	-6.190	-2.146
C7’	3.547	-5.919	-0.779
C8’	3.298	-4.649	-0.278
C9’	2.871	-3.588	-1.152
C1’	2.630	-2.271	-0.682
O2	0.616	-1.720	1.228
C2	1.889	-1.638	1.587
C3	2.203	-1.297	2.959
C4	3.466	-1.198	3.393
C10	4.527	-1.386	2.509
C5	5.911	-1.239	2.928
C6	6.955	-1.386	2.025
C7	6.689	-1.654	0.739
C8	5.376	-1.817	0.304
C9	4.296	-1.708	1.137
C1	2.919	-1.877	0.728
H3’	1.580	-1.054	-3.549
H4’	2.088	-3.138	-4.291
H5’	2.801	-5.469	-3.920
H6’	3.628	-7.035	-2.464
H7’	3.814	-6.598	-0.202
H8’	3.408	-4.482	0.631
H3	1.508	-1.140	3.556
H4	3.636	-1.006	4.287
H5	6.100	-1.044	3.817
H6	7.837	-1.298	2.311
H7	7.389	-1.733	0.131
H8	5.226	-2.008	-0.594

Table S1. (continued)



Solution Structure Coordinates			
Atom	**X coordinate**	**Y coordinate**	**Z coordinate**
BINOL 2			
O2’	-0.812	1.611	-1.261
C2’	0.104	2.510	-1.590
C3’	0.504	2.503	-2.955
C4’	1.441	3.381	-3.391
C10’	2.065	4.286	-2.541
C5’	3.079	5.174	-3.026
C6’	3.660	6.042	-2.146
C7’	3.353	6.032	-0.779
C8’	2.377	5.181	-0.278
C9’	1.672	4.280	-1.152
C1’	0.652	3.413	-0.682
O2	1.182	1.393	1.228
C2	0.474	2.455	1.587
C3	0.021	2.556	2.959
C4	-0.695	3.601	3.393
C10	-1.063	4.613	2.509
C5	-1.882	5.738	2.928
C6	-2.277	6.716	2.025
C7	-1.912	6.620	0.739
C8	-1.114	5.564	0.304
C9	-0.668	4.575	1.137
C1	0.166	3.467	0.728
H3’	0.123	1.896	-3.549
H4’	1.674	3.377	-4.291
H5’	3.336	5.160	-3.920
H6’	4.278	6.659	-2.464
H7’	3.807	6.602	-0.201
H8’	2.177	5.193	0.631
H3	0.233	1.876	3.556
H4	-0.947	3.652	4.287
H5	-2.146	5.804	3.817
H6	-2.794	7.436	2.311
H7	-2.194	7.265	0.131
H8	-0.873	5.530	-0.594

Table S1. (continued)



Solution Structure Coordinates			
Atom	**X coordinate**	**Y coordinate**	**Z coordinate**
BINOL 3			
O2’	-0.989	-1.509	-1.261
C2’	-2.226	-1.165	-1.590
C3’	-2.419	-0.815	-2.955
C4’	-3.648	-0.443	-3.391
C10’	-4.744	-0.354	-2.541
C5’	-6.020	0.080	-3.026
C6’	-7.062	0.149	-2.146
C7’	-6.900	-0.112	-0.779
C8’	-5.675	-0.532	-0.278
C9’	-4.543	-0.692	-1.152
C1’	-3.282	-1.142	-0.682
O2	-1.797	0.327	1.228
C2	-2.363	-0.816	1.587
C3	-2.224	-1.260	2.959
C4	-2.771	-2.403	3.393
C10	-3.464	-3.227	2.509
C5	-4.029	-4.499	2.928
C6	-4.678	-5.330	2.025
C7	-4.777	-4.966	0.739
C8	-4.261	-3.747	0.304
C9	-3.628	-2.866	1.137
C1	-3.085	-1.590	0.728
H3’	-1.703	-0.841	-3.549
H4’	-3.762	-0.239	-4.291
H5’	-6.136	0.309	-3.920
H6’	-7.906	0.376	-2.464
H7’	-7.621	-0.004	-0.202
H8’	-5.585	-0.711	0.631
H3	-1.741	-0.736	3.556
H4	-2.689	-2.646	4.287
H5	-3.954	-4.761	3.817
H6	-5.043	-6.137	2.311
H7	-5.195	-5.533	0.131
H8	-4.352	-3.521	-0.594
Yb	0.000	0.000	0.000

Figure S1. EXSY spectra of $K_3[Yb((S)\text{-BINOL})_3]$ (**2**) in the presence of about 1 eq. of (*S*)-BINOL in d_8-THF.