

SUPPORTING INFORMATION

Benzannulated *Tris*(2-mercapto-1-imidazolyl)hydroborato Ligands: Tetradentate κ^4 - S_3H Binding and Access to Monomeric Monovalent Thallium in an $[S_3]$ Coordination Environment

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Received xxxx xx, 2013.

Table 1. Cartesian coordinates for geometry optimized structure of $[\text{Tm}^{\text{Bu}^t\text{Benz}}]\text{Tl}$.

[Tm ^{Bu^tBenz}] ⁺ Tl ⁻			
-2831.79567939041 Hartrees			
Atom	x	y	z
Tl	-0.006958188	10.27295894	20.13067065
S	-2.271690225	9.838057642	18.37110855
N	-0.769949132	8.973006161	16.2631578
N	-2.121940516	7.38283907	17.07735336
B	0.003978959	10.27091241	15.87333384
H	0.00494627	10.26948754	14.67165914
C	-1.706716042	8.702401698	17.2111248
C	-0.554611984	7.818494721	15.51962821
C	0.330131643	7.60527368	14.45858176
H	0.976330158	8.399615489	14.10766447
C	0.360488882	6.343575876	13.87856696
H	1.038042795	6.147062546	13.05302381
C	-0.471077732	5.324872649	14.35842666
H	-0.434791727	4.340249864	13.90116677
C	-1.349055891	5.533794747	15.41887975
H	-1.958176793	4.710272394	15.74922982
C	-1.394380113	6.805447918	16.01435151
C	-3.187635436	6.735923849	17.94616135
C	-2.711152218	6.712376633	19.41280691
H	-2.577830708	7.715636737	19.81225465
H	-1.764179567	6.168524553	19.49272815

H	-3.456904672	6.190871087	20.02193096
C	-3.449261868	5.275675457	17.54130964
H	-3.81275994	5.183389007	16.51556057
H	-4.236687572	4.89853729	18.19975802
H	-2.574144427	4.638296313	17.68592662
C	-4.519396741	7.492686252	17.7668194
H	-4.441258484	8.537066827	18.06358454
H	-5.287695946	7.012991754	18.3822659
H	-4.842698492	7.444775094	16.72149011
S	1.514329873	8.527574699	18.38163316
N	1.515571647	10.2477123	16.26236489
N	3.56923055	9.865535253	17.07286198
C	2.217400388	9.573827663	17.21290924
C	2.410194605	10.9994385	15.50955684
C	2.154494013	11.86436223	14.44160227
H	1.143268004	12.03032066	14.09300182
C	3.234459868	12.50827099	13.85133822
H	3.067505616	13.18648812	13.01990061
C	4.532772992	12.29280757	14.32829473
H	5.369380158	12.80626166	13.86325758
C	4.788832322	11.43620724	15.39593932
H	5.806962592	11.31629304	15.7238846
C	3.707747679	10.77426141	16.00160451
C	4.661954101	9.266783872	17.94289704
C	4.449981152	9.703264972	19.40691045
H	3.514355281	9.323493775	19.81222616
H	4.451220746	10.79587699	19.47838067

H	5.275035227	9.320184878	20.01658728
C	6.059036484	9.760396941	17.53011231
H	6.316310085	9.483620748	16.50534673
H	6.778849432	9.267882009	18.1896706
H	6.179411555	10.83732455	17.66696198
C	4.663441123	7.733574444	17.77541423
H	3.717271708	7.286917679	18.07609755
H	5.460527405	7.308163528	18.39419312
H	4.864847427	7.467724028	16.73216487
S	0.760439179	12.44918356	18.37702245
N	-0.732089007	11.59067654	16.26057761
N	-1.433232673	13.55528069	17.07771794
C	-0.501326003	12.53355379	17.2130394
C	-1.83485926	11.98602273	15.51280175
C	-2.457276412	11.33141694	14.44616332
H	-2.093060391	10.37454622	14.09485625
C	-3.55926473	11.94143937	13.8607507
H	-4.06450685	11.45706118	13.03054229
C	-4.024278183	13.17153519	14.34078792
H	-4.890187256	13.63716075	13.87897291
C	-3.409042294	13.82234204	15.40719746
H	-3.815760335	14.76285128	15.73676113
C	-2.291871917	13.21947747	16.008909
C	-1.467211082	14.79459567	17.95612764
C	-1.737927483	14.38222009	19.41755325
H	-0.93632074	13.76673	19.82059692
H	-2.680083159	13.82836248	19.48438869

H	-1.827482215	15.28404113	20.03224853
C	-2.59827184	15.75345215	17.54894826
H	-2.48877462	16.12084084	16.52618882
H	-2.536832779	16.61984592	18.21330399
H	-3.588534871	15.31257798	17.68292435
C	-0.144413054	15.57075657	17.79383094
H	0.718499801	14.97856202	18.09345052
H	-0.181042503	16.47120313	18.41595488
H	-0.015280144	15.8826992	16.75192388