

Supporting Information

for

Preparation of RSn(I)-Sn(I)R with Two Unsymmetrically Coordinated Sn(I) Atoms and Subsequent Gentle Activation of P₄

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Content:

(S1). Solid-state NMR of **2**

(S2). Computational details of **2**

(S1). Solid-state NMR:

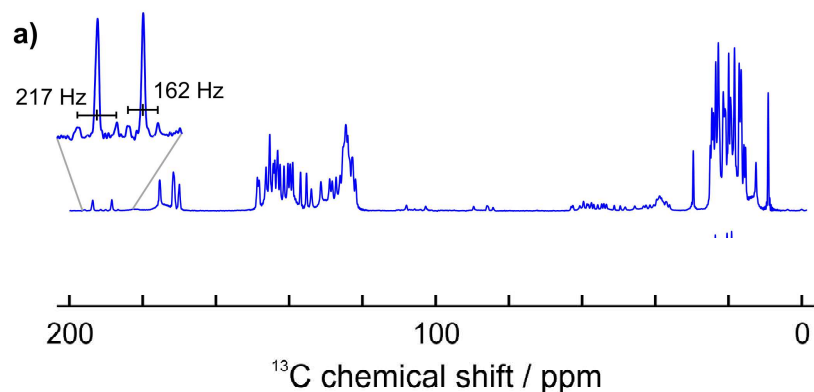


Figure S1. ^{13}C solid-state cross-polarization NMR spectrum of a bis(stannylene) **2**. The excerpt highlights the one-bond carbon-tin J couplings. The integrals of the satellite peaks (18.9% and 15.9% of total volume) correspond to the combined natural abundance of ^{117}Sn (7.61%) and ^{119}Sn (8.58%). The spectra were recorded at 8.2 KHz MAS on a 9.4 T spectrometer.

(S2). Computational Results (Structures and Density Plots)

Optimized B3LYP/def2-SVP structure of compound **2**

160

Sn	-8.590860	0.437721	-1.692053
Sn	-7.646708	2.993281	-0.329428
C	0.363596	0.628180	0.035699
H	1.309455	0.321064	-0.418047
C	-0.471319	-0.320967	0.629953
H	-0.164177	-1.368924	0.633831
C	-1.684901	0.044084	1.224330
C	-2.072327	1.413780	1.196738
C	-1.226648	2.389617	0.604843
C	-0.015786	1.968424	0.034131
H	0.646596	2.710658	-0.419366
C	-2.561255	-0.979902	1.943346
H	-3.610546	-0.679517	1.787947
C	-2.422410	-2.410998	1.407342
H	-2.577506	-2.453167	0.316868
H	-3.165840	-3.068469	1.887384
H	-1.430863	-2.842720	1.622914

C	-2.303396	-0.939343	3.462665
H	-2.985246	-1.621761	3.997451
H	-2.452566	0.075528	3.859823
H	-1.268069	-1.245215	3.689463
C	-1.572406	3.877354	0.640431
H	-2.620497	3.971071	0.958698
C	-0.722069	4.611330	1.694867
H	-0.850884	4.158852	2.690809
H	-1.010033	5.674266	1.763283
H	0.351053	4.567125	1.442721
C	-1.459370	4.555006	-0.735820
H	-1.801460	5.601758	-0.679096
H	-2.072469	4.037174	-1.490858
H	-0.420400	4.572629	-1.104787
C	-8.955503	-2.179555	0.623032
C	-9.921148	-3.050096	0.047820
C	-10.865880	-3.649689	0.893567
H	-11.612630	-4.323835	0.465046
C	-10.871734	-3.409429	2.265759
H	-11.613624	-3.892878	2.907123
C	-9.924373	-2.546126	2.813509
H	-9.932511	-2.360454	3.889980
C	-8.958830	-1.911733	2.016655
C	-9.961120	-3.373573	-1.446601
H	-9.181954	-2.778315	-1.943677
C	-11.300718	-2.971369	-2.090211
H	-12.144742	-3.540982	-1.667436
H	-11.278790	-3.168018	-3.175111
H	-11.506653	-1.900068	-1.944007
C	-9.651278	-4.858664	-1.717003
H	-10.423577	-5.517461	-1.286532
H	-8.684478	-5.160446	-1.284372
H	-9.612856	-5.055393	-2.801309
C	-7.925180	-0.995058	2.667036
H	-7.511573	-0.351190	1.874881
C	-6.757649	-1.796590	3.276731
H	-7.113145	-2.460315	4.083300
H	-6.004793	-1.115449	3.706389
H	-6.251291	-2.425500	2.530225
C	-8.534681	-0.071631	3.732577
H	-9.387695	0.498612	3.333949
H	-7.781284	0.648640	4.083932
H	-8.885107	-0.632872	4.614736
C	-8.344790	2.788488	-4.636571
C	-7.755271	4.079207	-4.769669
C	-8.507632	5.092773	-5.383712
H	-8.067959	6.087970	-5.488393
C	-9.791461	4.864394	-5.871431
H	-10.353575	5.672995	-6.345953
C	-10.346459	3.591360	-5.757784
H	-11.346196	3.405751	-6.157496
C	-9.649759	2.541076	-5.146464
C	-6.335477	4.420077	-4.306955
H	-5.908134	3.528667	-3.824744

C	-6.309216	5.548619	-3.261695
H	-6.693797	6.495002	-3.676134
H	-5.275491	5.734007	-2.925042
H	-6.910174	5.290887	-2.378056
C	-5.424409	4.794629	-5.494226
H	-5.421717	4.027330	-6.282703
H	-4.385545	4.936584	-5.153390
H	-5.749042	5.740023	-5.959586
C	-10.274904	1.148235	-5.115644
H	-9.682784	0.535843	-4.419259
C	-10.189143	0.475043	-6.499753
H	-10.769744	1.034090	-7.252977
H	-10.588953	-0.551766	-6.459699
H	-9.149076	0.418961	-6.859864
C	-11.718494	1.146040	-4.587833
H	-11.781201	1.622257	-3.597179
H	-12.086240	0.111489	-4.489367
H	-12.410313	1.676353	-5.262811
C	-10.734260	3.873261	0.508949
C	-11.788686	2.922163	0.498200
C	-13.027302	3.312041	-0.032657
H	-13.851782	2.595261	-0.043164
C	-13.231239	4.590798	-0.546652
H	-14.205019	4.870024	-0.957562
C	-12.184570	5.508904	-0.536379
H	-12.346880	6.510430	-0.941896
C	-10.924448	5.179029	-0.015216
C	-9.830059	6.245845	-0.009965
H	-8.896679	5.770645	0.326497
C	-10.151090	7.385091	0.976283
H	-11.063732	7.928448	0.678563
H	-9.324465	8.114756	1.009197
H	-10.310244	7.009671	1.999090
C	-9.562123	6.804460	-1.418138
H	-9.337555	5.999918	-2.133745
H	-8.700943	7.492542	-1.399452
H	-10.426895	7.368351	-1.805693
C	-11.633622	1.514848	1.073478
H	-10.555106	1.316569	1.173322
C	-12.213449	0.427794	0.152980
H	-11.952211	-0.570362	0.538326
H	-11.813472	0.510716	-0.868579
H	-13.313351	0.479157	0.096138
C	-12.263437	1.401373	2.476407
H	-13.349551	1.591311	2.436084
H	-11.828358	2.118442	3.187613
H	-12.113652	0.388150	2.883966
C	-6.818632	2.805563	1.743397
C	-7.757089	3.309895	2.704738
C	-7.385061	3.499991	4.053608
H	-8.099096	3.896788	4.776707
C	-6.102808	3.182015	4.483417
H	-5.820034	3.322768	5.529639
C	-5.175436	2.695158	3.563619

H	-4.158927	2.451325	3.875799
C	-5.500414	2.518082	2.204808
C	-4.372819	2.048624	1.321360
C	-4.604861	1.914834	-0.160317
H	-4.844946	2.896344	-0.605353
H	-5.449420	1.239101	-0.369626
H	-3.717564	1.518989	-0.670727
C	-9.115756	3.674531	2.282154
C	-10.064828	4.291079	3.282458
H	-11.041497	4.507496	2.836380
H	-9.647323	5.231207	3.677064
H	-10.215888	3.620790	4.142222
C	-6.653475	-0.364211	-2.362044
C	-6.010162	0.077163	-3.546244
C	-4.793183	-0.506397	-3.946077
H	-4.280795	-0.162740	-4.846306
C	-4.213463	-1.535956	-3.200250
H	-3.255957	-1.962681	-3.506663
C	-4.882581	-2.041810	-2.088030
H	-4.444457	-2.883838	-1.549589
C	-6.108324	-1.479885	-1.673954
C	-6.655304	1.114516	-4.395602
C	-6.123590	1.312015	-5.798906
H	-6.763553	1.989944	-6.375777
H	-6.072513	0.343755	-6.321184
H	-5.104383	1.728459	-5.786122
C	-6.904594	-2.111524	-0.600119
C	-6.446974	-3.444268	-0.051735
H	-7.135626	-3.829391	0.709110
H	-5.445801	-3.351105	0.397467
H	-6.366946	-4.187784	-0.861346
N	-3.239598	1.800101	1.874192
N	-9.447042	3.496827	1.025685
N	-7.679762	1.748518	-3.929162
N	-8.012260	-1.534513	-0.235649

Optimized B3LYP/def2-SVP structure of 3- and 4-coordination model

88

C	-8.812128	0.446639	-1.526536
C	-8.175817	1.575027	-0.952020
C	-6.784316	1.521546	-0.689240
C	-6.061761	0.342038	-0.954121
C	-6.706453	-0.776700	-1.487788
C	-8.070489	-0.723236	-1.783638
Sn	-9.298446	3.430443	-0.635269
N	-10.851685	1.656896	-1.558123
C	-10.252502	0.543397	-1.854936
C	-10.929554	-0.613554	-2.552873
C	-6.127742	2.730038	-0.140091

N	-6.885309	3.756956	0.096164
C	-6.436308	4.966614	0.664968
C	-5.973292	5.025527	1.993056
C	-5.594867	6.247520	2.554528
C	-5.673633	7.426092	1.805760
C	-6.145882	7.373985	0.489857
C	-6.534378	6.158181	-0.076750
H	-5.933200	4.108609	2.585354
H	-6.913150	6.114133	-1.099900
Sn	-9.833041	2.938350	2.316426
N	-11.834062	4.034704	2.180802
C	-12.897472	3.278860	2.292469
C	-14.289693	3.857038	2.365537
C	-11.363870	1.293504	2.311521
C	-12.694010	1.826627	2.373860
C	-13.813941	0.978075	2.506147
C	-13.650416	-0.401192	2.554962
C	-12.366298	-0.940194	2.486736
C	-11.224038	-0.121980	2.382258
C	-9.903744	-0.848353	2.366897
N	-9.930723	-2.129776	2.275725
C	-8.822558	-2.973986	2.343696
C	-8.459611	-3.742400	1.218163
C	-7.399351	-4.646971	1.286626
C	-6.691623	-4.826882	2.481025
C	-7.058306	-4.084958	3.608353
C	-8.108280	-3.165857	3.545089
H	-9.025380	-3.614174	0.292315
H	-8.398952	-2.596744	4.431498
C	-8.625930	-0.052299	2.447526
C	-4.631141	2.728151	0.072097
C	-11.869594	5.444107	2.011774
C	-12.370815	6.014678	0.828602
C	-12.344356	7.400043	0.652938
C	-11.814820	8.230441	1.646510
C	-11.305820	7.663822	2.819113
C	-11.326290	6.278577	3.002576
H	-12.762419	5.363257	0.043980
H	-10.927744	5.831077	3.915750
C	-12.220032	1.914663	-1.770119
C	-12.593789	3.010355	-2.572937
C	-13.942236	3.324295	-2.757298
C	-14.939594	2.565383	-2.134266
C	-14.572980	1.487732	-1.321090
C	-13.226520	1.162575	-1.134956
H	-11.812515	3.601860	-3.054857
H	-12.946049	0.339234	-0.475103
H	-5.867384	-5.542910	2.534086
H	-7.127939	-5.224839	0.398292
H	-6.521336	-4.220967	4.551642
H	-14.215636	4.170711	-3.393857
H	-15.994129	2.813929	-2.280125
H	-15.339995	0.891529	-0.819613
H	-5.239738	6.276816	3.588057

H	-5.375610	8.380472	2.247028
H	-6.218263	8.290342	-0.102449
H	-12.732861	7.831834	-0.273467
H	-11.792261	9.314119	1.503682
H	-10.885629	8.303018	3.600277
H	-14.820623	1.394524	2.566552
H	-14.519083	-1.057296	2.653599
H	-12.211957	-2.020291	2.522452
H	-8.602577	0.572986	3.355295
H	-8.544192	0.615136	1.572313
H	-7.743965	-0.704557	2.450034
H	-14.270862	4.950747	2.443730
H	-14.828765	3.455393	3.237760
H	-14.871483	3.586153	1.468444
H	-4.991627	0.280046	-0.742620
H	-6.142640	-1.692937	-1.678279
H	-8.548181	-1.606997	-2.213103
H	-4.257521	3.723000	0.342114
H	-4.116005	2.395553	-0.842645
H	-4.347899	2.025542	0.873553
H	-11.935355	-0.348118	-2.898933
H	-11.017548	-1.479075	-1.875250
H	-10.335113	-0.939692	-3.419878

Optimized B3LYP/def2-SVP structure of 3- and 4-coordination model

88

C	-13.022853	-1.770576	-6.083922
C	-11.689836	-1.373754	-5.873429
C	-11.161365	-0.319217	-6.641314
C	-11.947446	0.307119	-7.611418
C	-13.265765	-0.104428	-7.831799
C	-13.797707	-1.145021	-7.063011
N	-10.940718	-1.977574	-4.841870
C	-9.854648	-2.663665	-5.030268
C	-9.299146	-2.988978	-6.396956
C	-9.160891	-3.166124	-3.822916
C	-9.715591	-2.861219	-2.554461
C	-9.090404	-3.377580	-1.391090
C	-7.902558	-4.127279	-1.503599
C	-7.349813	-4.395448	-2.758386
C	-7.983378	-3.931630	-3.914015
C	-9.738232	-3.148900	-0.080406
C	-9.145892	-3.790919	1.155259
Sn	-11.642172	-1.824963	-2.427829
N	-10.833198	-2.451043	-0.073351
C	-11.579238	-2.146783	1.079447
C	-12.919559	-2.574976	1.159790
C	-13.699654	-2.254544	2.273013
C	-13.167507	-1.488353	3.317108

C	-11.844315	-1.042384	3.232520
C	-11.054505	-1.363626	2.125357
Sn	-10.765213	1.084630	-2.580529
N	-12.691537	1.566021	-1.038948
C	-12.331543	1.894751	0.165288
C	-13.296848	2.360880	1.230089
C	-9.996548	1.435636	-0.559991
C	-8.602105	1.435329	-0.301314
C	-8.123623	1.767062	0.981838
C	-9.011612	2.130100	1.997651
C	-10.383774	2.182340	1.739673
C	-10.884332	1.838672	0.469665
C	-7.676239	1.132757	-1.415515
C	-6.185339	1.249661	-1.184231
N	-8.205223	0.846310	-2.566321
C	-7.472523	0.545392	-3.728223
C	-6.635360	-0.583290	-3.813643
C	-5.959898	-0.874586	-5.001871
C	-6.108803	-0.054492	-6.125324
C	-6.951679	1.060745	-6.051123
C	-7.634981	1.356324	-4.869601
C	-14.026427	1.496862	-1.486304
C	-14.951791	0.603518	-0.913297
C	-16.247766	0.507550	-1.425415
C	-16.641644	1.293215	-2.513150
C	-15.721753	2.173057	-3.093097
C	-14.421887	2.271051	-2.592599
H	-8.295391	2.224134	-4.808558
H	-6.537690	-1.244487	-2.949923
H	-14.638445	-0.031174	-0.081175
H	-13.696867	2.947968	-3.049856
H	-13.331742	-3.168327	0.340635
H	-10.032417	-0.987197	2.052102
H	-10.139095	0.016738	-6.454832
H	-13.437808	-2.576942	-5.474908
H	-5.575310	-0.282917	-7.051576
H	-7.078753	1.710058	-6.922275
H	-5.314264	-1.756447	-5.047380
H	-14.732808	-2.608812	2.324614
H	-13.780366	-1.239396	4.187505
H	-11.418923	-0.432690	4.034727
H	-11.524954	1.129840	-8.195209
H	-13.877370	0.388230	-8.592207
H	-14.828985	-1.471673	-7.221751
H	-16.953157	-0.195303	-0.973134
H	-17.655629	1.212672	-2.913196
H	-16.014487	2.784946	-3.950918
H	-11.058557	2.488146	2.541961
H	-8.630846	2.389856	2.988690
H	-7.053257	1.752720	1.201562
H	-5.831030	0.465170	-0.494563
H	-5.944523	2.218830	-0.719910
H	-5.618449	1.161789	-2.118371
H	-14.300172	2.530196	0.821512

H	-12.942200	3.298770	1.684510
H	-13.375554	1.613567	2.037391
H	-7.544271	-4.167705	-4.885546
H	-6.428451	-4.978215	-2.836222
H	-7.398573	-4.514438	-0.615275
H	-9.990891	-2.695581	-7.195538
H	-9.098090	-4.067891	-6.484687
H	-8.343224	-2.463715	-6.558666
H	-9.806234	-3.687618	2.024488
H	-8.174650	-3.333697	1.408245
H	-8.961770	-4.862222	0.980390

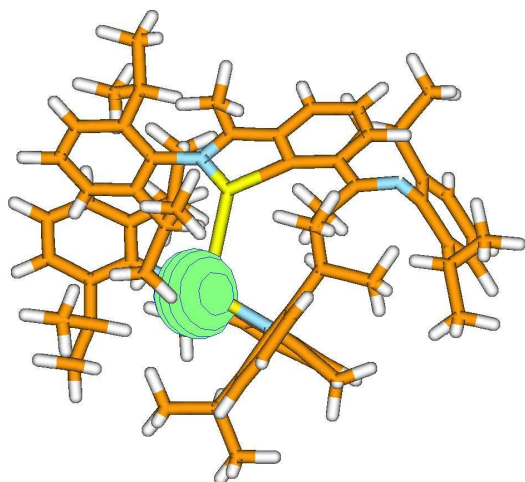


Figure S2. Isosurface plots of the two Sn NLMOs derived from the Sn NBO lone pairs in compound **2**.