Supplementary Material (ESI) for Dalton Transactions

Supplementary Materials

Basis	Sn-Sn (Å)	θ °	ω °
ECP	3.134	98.1	180
All E	2.987	99.3	180

Table 1: Comparison of an effective core potential and an all-electron basis for the PhSnSnPh system

Method	Sn-Sn (Å)	θ °	ω °
B3LYP	3.134	98.1	180
B3PW91	3.082	98.3	180

Table 2: Comparison of two different functionals for the model PhSnSnPh system

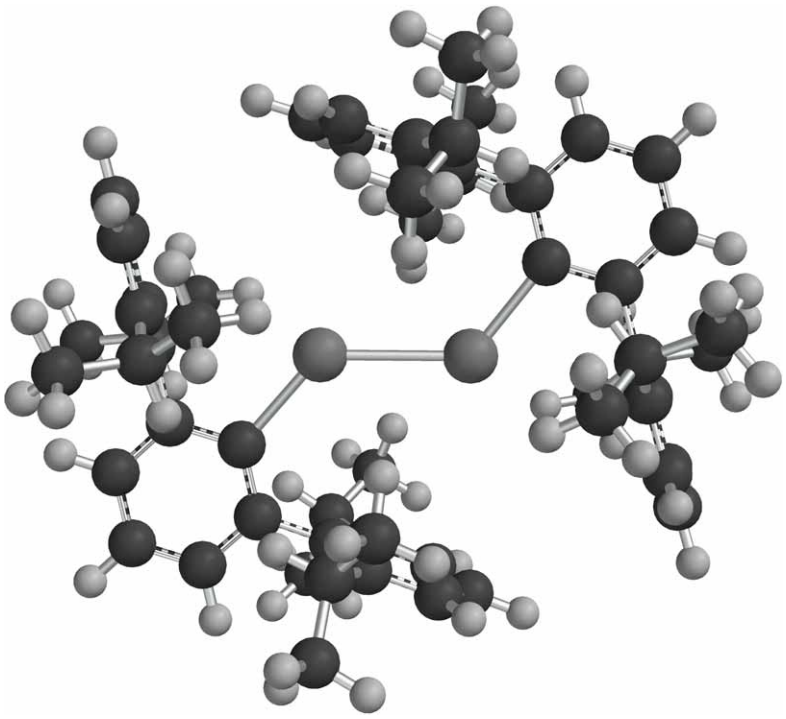

Figure 1: Fully optimized Ar'SnSnAr' structure

Coordinates for Optimized Structure (in Å)

Atom	X	Y	Z
Sn	8.965983	7.834027	.736557
C	8.439439	6.417413	2.425047
C	9.197124	5.340727	2.936034
C	8.662097	4.543194	3.960536
C	7.393484	4.798358	4.480573
C	6.641390	5.861898	3.981257
C	7.156008	6.674502	2.961212
C	6.334480	7.826556	2.439311
C	5.358026	7.602833	1.433162

C	4.581765	8.683060	.991109
C	4.763280	9.959683	1.512411
C	5.723532	10.177673	2.496669
C	6.515854	9.129911	2.982588
C	5.106830	6.218874	.834239
C	5.176016	6.230835	-.704377
C	3.763620	5.638490	1.320184
C	7.489898	9.388262	4.132934
C	6.761973	9.270605	5.489494
C	8.215863	10.742374	4.035918
C	10.567748	5.025176	2.406311
C	11.708385	5.601103	3.016334
C	12.975455	5.300287	2.500927
C	13.124728	4.453189	1.406162
C	12.002057	3.867886	.827975
C	10.714849	4.138526	1.309936
C	11.604000	6.479427	4.264508
C	12.204963	5.758529	5.488838
C	12.239349	7.870296	4.080947
C	9.516746	3.412688	.698600
C	9.451837	3.534613	-.833959
C	9.504573	1.932977	1.133787
H	9.249255	3.713940	4.348030
H	6.992119	4.171016	5.272131
H	5.651242	6.065306	4.382857
H	3.825297	8.521024	.227992
H	4.152373	10.785807	1.156882
H	5.850757	11.177088	2.900966
H	5.894171	5.548380	1.189210
H	4.358818	6.814967	-1.143996
H	5.095702	5.208966	-1.092752
H	6.123106	6.658111	-1.053169
H	3.738813	5.553410	2.412250
H	3.604184	4.639639	.896127
H	2.922741	6.272132	1.014444
H	8.254487	8.604940	4.101667
H	5.949580	10.004699	5.558445
H	7.458601	9.456701	6.315774
H	6.329696	8.274555	5.628497
H	8.677660	10.887683	3.053710
H	9.007928	10.792860	4.792099
H	7.538958	11.585104	4.220469
H	13.857959	5.734507	2.962669
H	14.114531	4.243533	1.009503
H	12.128053	3.189550	-.011366
H	10.542530	6.636178	4.475631

H	11.733597	4.781509	5.642835
H	12.059059	6.354900	6.397514
H	13.282158	5.593012	5.367107
H	12.117753	8.463778	4.996086
H	11.768903	8.417485	3.256686
H	13.314211	7.805648	3.872071
H	8.610747	3.877002	1.098432
H	10.322762	3.079801	-1.321237
H	9.404858	4.584407	-1.138889
H	8.558751	3.026311	-1.217688
H	8.618866	1.423039	.736360
H	9.491731	1.840703	2.225384
H	10.391514	1.405067	.763185
Sn	11.378548	7.982468	-.738482
C	11.991674	9.351235	-2.429220
C	11.187737	10.317852	-3.071988
C	11.726139	11.077349	-4.122520
C	13.043089	10.888288	-4.542189
C	13.838725	9.928783	-3.916037
C	13.322408	9.159131	-2.863907
C	14.191059	8.126994	-2.193126
C	14.921794	8.476051	-1.024942
C	15.732312	7.505274	-.420813
C	15.841166	6.225015	-.954694
C	15.134955	5.891244	-2.107318
C	14.303483	6.821286	-2.744358
C	14.928439	9.898852	-.466018
C	14.618872	9.956674	1.041389
C	16.273152	10.590537	-.774504
C	13.596131	6.423926	-4.041577
C	14.608344	6.320323	-5.202465
C	12.786730	5.118725	-3.913419
C	9.759036	10.546915	-2.667378
C	8.727466	9.789654	-3.280719
C	7.399506	10.046214	-2.919944
C	7.084412	11.016929	-1.971993
C	8.101349	11.754344	-1.373093
C	9.444579	11.541767	-1.708749
C	9.030172	8.743902	-4.355629
C	8.771222	9.322085	-5.762467
C	8.258932	7.426073	-4.159479
C	10.512191	12.433810	-1.074173
C	10.487312	12.391215	.465447
C	10.381560	13.882843	-1.586785
H	11.102021	11.821672	-4.611364
H	13.446399	11.483843	-5.356888

H	14.865866	9.774893	-4.239331
H	16.297823	7.762183	.470345
H	16.485693	5.489627	-.479275
H	15.239305	4.893105	-2.524035
H	14.151467	10.466978	-.985516
H	15.402582	9.476847	1.639581
H	14.548297	10.999715	1.370688
H	13.668152	9.463038	1.274363
H	16.476227	10.603990	-1.851038
H	16.261479	11.627920	-.418040
H	17.107914	10.076442	-.282730
H	12.891185	7.219131	-4.301203
H	15.354003	5.540314	-5.008213
H	14.094403	6.069744	-6.138315
H	15.142423	7.265332	-5.351949
H	12.040806	5.178727	-3.112812
H	12.257141	4.915457	-4.851709
H	13.430582	4.255753	-3.707930
H	6.597345	9.482270	-3.387286
H	6.047144	11.200202	-1.703901
H	7.850400	12.513438	-.637084
H	10.095697	8.501022	-4.291645
H	9.365869	10.224655	-5.938983
H	9.028859	8.587584	-6.535679
H	7.714588	9.588508	-5.888982
H	8.575468	6.693783	-4.911593
H	8.450322	7.000004	-3.169166
H	7.176690	7.558897	-4.271628
H	11.493097	12.066789	-1.390455
H	9.534904	12.751808	.872606
H	10.643868	11.371522	.832692
H	11.282375	13.026951	.873925
H	11.174719	14.514523	-1.168724
H	10.453377	13.923642	-2.679400
H	9.417391	14.318398	-1.299317