Electronic Supplementary Information for Dalton Transactions

Synthetic, structural and computational studies on adducts of the 4,1,2-SnC_2B_{10} supraicosahedral stannacarborane

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Electronic Supplementary Information

Additional Figures:

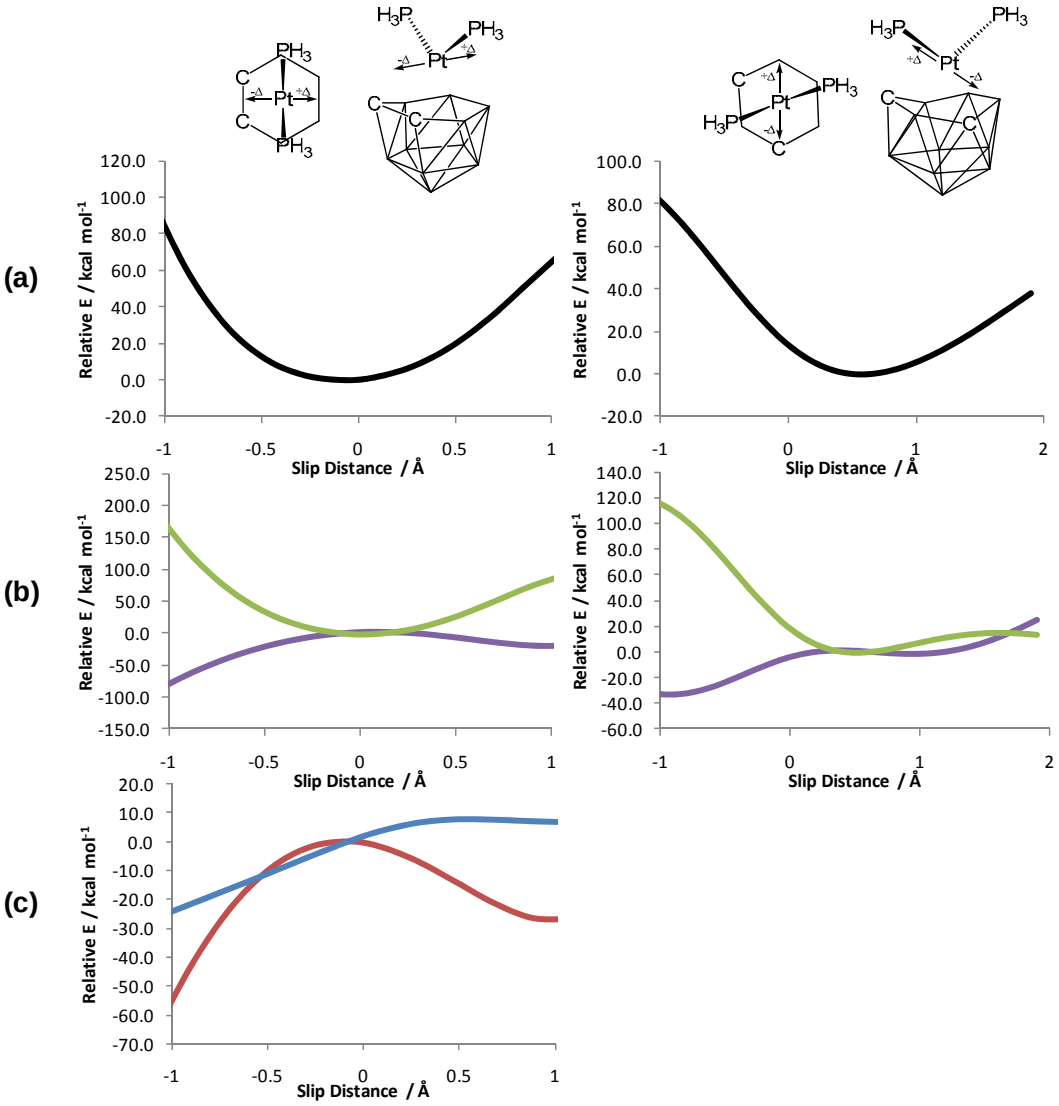

Figure 11a – Includes Plot (c) (a' (red) and a" (blue) orbital interaction terms *vs.* *Δ*) for model **E.**

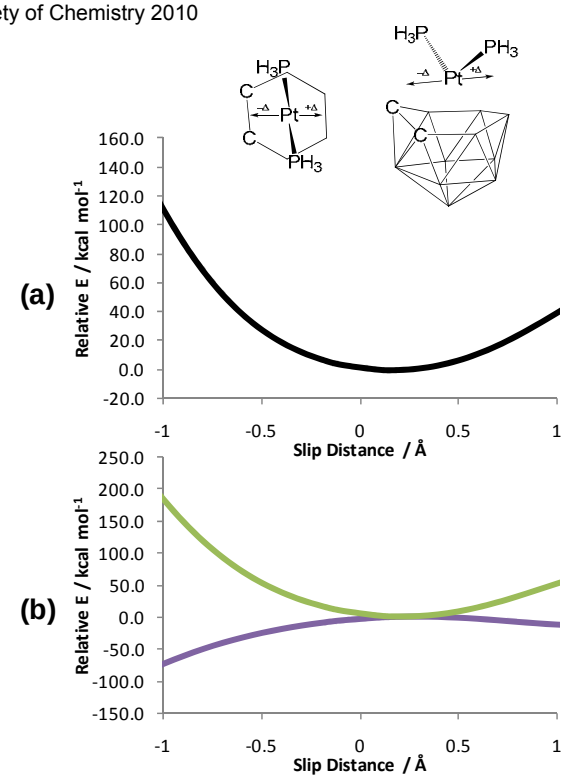

Figure 11b - Energy decomposition analyses for $\mathbf{E}_{C_1}$ for comparison with model **E** where C_s symmetry is enforced. Plots are (a) total interaction energy, (b) steric (green) and orbital (purple) interaction energy terms *vs.* Δ.

Optimised energies and atomic coordinates for the computational model compounds **A**-**F**:

A

BP86 Energy = -335.457500
Enthalpy 0K = -335.288400
Enthalpy 298K = -335.277312
Free Energy 298K = -335.323920
25

C	-0.140799	1.615739	-0.527911
C	0.224709	0.614796	-1.530973
B	0.222454	1.530475	0.975894
Sn	-1.639267	-0.269701	0.305507
B	1.630179	1.431184	-0.446620
B	0.264899	-1.079824	-1.199674
B	0.408866	-0.142894	1.757114
B	1.827985	0.793209	1.336450
B	1.751934	-0.136807	-1.530468
B	0.338384	-1.538472	0.576160
B	2.652732	0.019402	-0.014239
B	1.800960	-1.515649	-0.445295
B	1.880192	-0.971998	1.269014
H	-0.590108	2.535765	-0.918946
H	-0.026578	0.902012	-2.558828
H	-0.080398	2.488621	1.630013
H	2.115278	2.429549	-0.889434
H	-0.185913	-1.739512	-2.094587
H	0.004113	-0.173069	2.889520
H	2.416731	1.475394	2.126651
H	2.247653	-0.125552	-2.619223
H	-0.166635	-2.585799	0.902592
H	3.831431	0.191168	-0.138153
H	2.374257	-2.510196	-0.782676
H	2.510453	-1.610861	2.060600

B

BP86 Energy = -830.863182
Enthalpy 0K = -830.539264
Enthalpy 298K = -830.517460
Free Energy 298K = -830.590377
45

C	0.631469	-0.212141	3.392619
C	1.831032	0.052599	2.647690
B	-0.581515	-1.125584	2.979215
Sn	-0.186278	0.867003	0.905804
B	0.917667	-1.991527	3.602757
B	2.201652	-0.454889	1.174401
B	-0.661335	-1.607844	1.175096
B	-0.249763	-2.764686	2.448360
B	2.525482	-1.611667	2.547660
B	0.822821	-1.260869	0.202287
B	1.526831	-3.030042	2.334041
B	2.171285	-2.186908	0.877761
B	0.524332	-2.879480	0.846849
H	0.495929	0.369410	4.313709
H	2.509644	0.806318	3.067886
H	-1.542633	-1.001982	3.693354
H	1.083442	-2.241681	4.763036
H	3.138524	0.136547	0.695508
H	-1.763738	-1.647845	0.683867

H	-1.028089	-3.604903	2.805388
H	3.586978	-1.643200	3.103751
H	0.789592	-1.074357	-0.987705
H	2.016346	-4.058418	2.712217
H	3.029769	-2.640467	0.173430
H	0.284738	-3.806689	0.124738
N	0.583724	1.664811	-1.471565
C	1.875373	2.000537	-1.654656
C	2.353165	2.563464	-2.845378
C	1.438073	2.791124	-3.882851
C	0.095616	2.440823	-3.698145
C	-0.309574	1.867700	-2.473868
C	-1.713220	1.438143	-2.210781
C	-2.750071	1.616253	-3.151250
C	-4.040241	1.165733	-2.849810
C	-4.276080	0.547798	-1.613874
C	-3.201313	0.417803	-0.724981
N	-1.956242	0.848310	-1.010267
H	2.544332	1.786325	-0.813313
H	3.413134	2.808889	-2.951433
H	1.764569	3.230300	-4.830497
H	-0.621419	2.604339	-4.505897
H	-2.556880	2.098732	-4.112009
H	-4.849743	1.294748	-3.574759
H	-5.265115	0.171999	-1.339174
H	-3.325301	-0.062610	0.251613

C

BP86 Energy = -442.851269
Enthalpy 0K = -442.643256
Enthalpy 298K = -442.626747
Free Energy 298K = -442.686957
31

C	-0.471550	-0.455694	-1.532024
C	-1.435129	0.389786	-0.748389
Pt	0.738419	2.053869	-1.311494
B	1.233484	-0.110532	-1.012350
B	0.257836	-1.629367	-0.649617
B	-1.484344	-1.291032	-0.435776
B	-0.535882	1.441978	0.426594
B	1.220177	0.907647	0.517573
B	1.195590	-0.845416	0.675029
B	-0.447923	-1.443544	1.003183
B	-1.562567	-0.032077	0.830834
B	0.055807	0.154673	1.601963
H	-0.644270	-0.569028	-2.605025
H	-2.265400	0.853414	-1.286634
H	2.110983	-0.459842	-1.759862
H	0.619667	-2.629692	-1.195489
H	-2.388724	-1.970837	-0.814371
H	-1.132433	2.386055	0.877861
H	2.142475	1.511111	1.000566
H	2.140714	-1.429295	1.123846
H	-0.648486	-2.360350	1.745728
H	-2.585592	0.182723	1.411202
H	0.102278	0.359307	2.781613
P	2.173100	2.231844	-3.200807
P	-0.142566	4.263692	-1.317576
H	1.800710	1.582003	-4.430816
H	2.595448	3.485265	-3.775375
H	3.467701	1.629471	-3.050627
H	-1.500557	4.478626	-1.746005
H	-0.247192	4.889104	-0.029434
H	0.452645	5.365404	-2.032786

D

BP86 Energy = -442.875377
Enthalpy 0K = -442.666635
Enthalpy 298K = -442.650395
Free Energy 298K = -442.709826
31

C	-0.700371	-0.215872	-1.528466
Pt	0.505654	1.932323	-1.434052
B	-1.253075	0.982728	-0.395315
B	-1.620521	-0.810085	-0.288409
B	-0.146455	-1.641338	-0.810143
B	0.954007	-0.304209	-1.336156
C	-0.081367	1.252411	0.861876
B	-1.229851	0.116588	1.220199
B	-0.467542	-1.478273	0.912949
B	1.192871	-1.098807	0.249879
B	1.369888	0.682264	0.269806
B	0.477511	-0.161286	1.599357
H	-1.164122	-0.264200	-2.515813
H	-2.228319	1.662418	-0.560269
H	-2.731088	-1.195669	-0.504868
H	-0.164018	-2.656445	-1.441512
H	1.708656	-0.549801	-2.237284
H	-0.137369	2.171267	1.449089
H	-2.074747	0.361177	2.029652
H	-0.736146	-2.439817	1.573142
H	2.138316	-1.809524	0.441608
H	2.431681	1.165221	0.554744
H	0.911561	-0.105162	2.711934
P	-0.775983	3.772871	-2.232729
P	2.576794	2.540784	-2.344147
H	-0.198029	4.825117	-3.028742
H	-1.915369	3.504645	-3.070035
H	-1.450256	4.607910	-1.273932
H	2.736078	3.741222	-3.122773
H	3.208546	1.619243	-3.249449
H	3.677482	2.731568	-1.438604

E

BP86 Energy = -468.287182
Enthalpy 0K = -468.067269
Enthalpy 298K = -468.050263
Free Energy 298K = -468.110607
NImag = 1 (-257.2 cm-1)
33

C	-0.915220	0.707998	1.706878
C	-0.915220	-0.707997	1.706878
B	-0.986743	1.622012	0.299045
Pt	0.632954	0.000001	0.005689
B	-2.545285	0.975674	1.017488
B	-0.986742	-1.622010	0.299045

B	-0.914821	0.891516	-1.459718
B	-2.426684	1.468739	-0.705182
B	-2.545285	-0.975672	1.017488
B	-0.914820	-0.891515	-1.459718
B	-3.347107	0.000001	-0.189053
B	-2.426683	-1.468738	-0.705182
B	-2.428005	0.000001	-1.715667
H	-0.621750	1.253875	2.610552
H	-0.621749	-1.253873	2.610552
H	-0.607030	2.740451	0.537704
H	-3.129791	1.572795	1.879177
H	-0.607029	-2.740449	0.537704
H	-0.413149	1.600681	-2.291848
H	-2.966840	2.475472	-1.068807
H	-3.129790	-1.572794	1.879177
H	-0.413149	-1.600679	-2.291848
H	-4.543735	0.000000	-0.111968
H	-2.966839	-2.475471	-1.068807
H	-2.978145	0.000001	-2.780331
P	2.218974	-1.766527	-0.100710
P	2.218973	1.766530	-0.100710
H	2.357424	-2.703270	0.983276
H	3.613266	-1.490649	-0.323004
H	2.004950	-2.703523	-1.166227
H	2.357423	2.703273	0.983276
H	3.613265	1.490653	-0.323004
H	2.004949	2.703526	-1.166227

E_{C_1}

BP86 Energy = -468.298878
Enthalpy 0K = -468.078023
Enthalpy 298K = -468.060449
Free Energy 298K = -468.121471
33

C	-0.727196	3.031623	1.408031
C	-0.349114	3.072940	0.014264
B	-0.293873	1.873508	2.382878
Pt	1.543485	3.236565	2.146419
B	-1.059700	1.458256	0.497590
B	1.474761	2.784767	-0.100084
B	0.118006	1.840699	-0.923247
B	-0.096678	0.256182	1.586978
B	1.342882	0.973948	2.328571
B	2.408235	1.544761	0.967311
B	0.096865	0.234523	-0.168333
B	1.657571	1.045253	-0.560897
B	1.508455	-0.001700	0.866112
H	-1.533757	3.716985	1.696229
H	-0.830868	3.850252	-0.588287
H	-0.879143	1.863631	3.437192
H	-2.236721	1.368089	0.313429
H	-0.158075	2.057354	-2.068053
H	-0.744927	-0.600485	2.121465
H	1.679081	0.560222	3.407265
H	1.991973	3.645537	-0.763431
H	3.609143	1.614039	0.945790
H	-0.401015	-0.630656	-0.832016
H	2.067784	-1.060187	0.916483
H	2.290845	0.745467	-1.533640
P	1.261605	3.756009	4.470721
P	2.980944	5.051361	1.582439
H	0.005558	4.258621	4.959777
H	2.130697	4.686810	5.141750
H	1.406693	2.642477	5.363149
H	2.530267	6.131279	0.743010
H	4.147470	4.688475	0.828512
H	3.622302	5.844574	2.598709

F

BP86 Energy = -468.317128
Enthalpy 0K = -468.095821
Enthalpy 298K = -468.078100
Free Energy 298K = -468.140640
33

C	-0.699112	-1.431500	0.897133
B	-0.975903	-1.628844	-0.642592
B	-0.998927	-0.191696	1.839852
Pt	0.685319	0.002849	0.083640
B	-2.418062	-1.104984	1.037066
C	-1.558542	-0.503550	-1.672224
B	-0.945032	1.362947	0.766178
B	-2.448919	0.707415	1.470633
B	-2.846342	-1.163929	-0.869631
B	-1.128146	1.024708	-1.135728
B	-3.471851	0.072988	0.174836
B	-2.845384	0.501101	-1.443018
B	-2.482130	1.573701	-0.084153
H	-0.301698	-2.322409	1.394157
H	-0.639814	-2.668630	-1.149038
H	-0.703437	-0.281522	2.998451
H	-2.942838	-1.979077	1.666336
H	-1.378184	-0.802519	-2.709095
H	-0.482719	2.396877	1.180453
H	-2.965832	1.210121	2.427884
H	-3.448336	-2.088868	-1.330504
H	-0.608035	1.763455	-1.928761
H	-4.646066	0.027893	0.411861
H	-3.460525	0.858278	-2.404216
H	-2.937370	2.682582	-0.120993
P	2.480385	-1.590429	-0.216365
P	1.990498	1.926615	-0.233413
H	2.437696	-2.805791	0.551036
H	3.847253	-1.236086	0.061419
H	2.698935	-2.191042	-1.506196
H	3.388936	1.835153	-0.559874
H	1.570698	2.845771	-1.251012
H	2.072484	2.822425	0.882876