Supplemental Material to

Alkylthio Bridged 44 cve Triangular Platinum Clusters: Syntheses, Oxidation, Degradation, Ligand Substitution and Quantum Chemical Calculations

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ENERGIES AND CARTESIAN COORDINATES OF ATOM POSITIONS OF CALCULATED MOLECULES

1. $[\{Pt(PPh_3)\}_3(\mu\text{-}SMe)_3]^+$ (4a')

SCF energy E(RmPW+HF–PW91)	–4769.0190131 a.u.
Zero-point vibrational energies	606.45 kcal/mol
Sum of electronic and zero-point energies	–4768.052571 a.u.
Sum of electronic and thermal energies	–4767.985554 a.u.
Sum of electronic and thermal enthalpies	–4767.984610 a.u.
Sum of electronic and thermal free energies	–4768.168502 a.u.

	x	y	z
Pt	0.014931	1.693357	0.088278
Pt	–1.473956	–0.833748	0.088278
Pt	1.459025	–0.859609	0.088278
S	–2.280429	1.334147	0.168603
S	–0.015190	–2.641983	0.168603
S	2.295620	1.307836	0.168603
C	–3.005200	1.706650	–1.470386
C	0.024597	–3.455904	–1.470386
C	2.980602	1.749254	–1.470386
P	0.000000	3.969239	0.074017

P	–3.437462	–1.984619	0.074017
P	3.437462	–1.984619	0.074017
H	–3.978260	1.210386	–1.521669
H	–3.139077	2.788190	–1.547633
H	–2.359164	1.361282	–2.277838
H	0.940905	–4.050467	–1.521669
H	–0.845105	–4.112616	–1.547633
H	0.000677	–2.723737	–2.277838
H	3.037355	2.840081	–1.521669
H	3.984182	1.324426	–1.547633
H	2.358487	1.362454	–2.277838
C	4.507808	–1.426704	–1.289523
C	5.810642	–0.960536	–1.080758
C	3.971071	–1.420448	–2.588731
C	6.568066	–0.503006	–2.159527
H	6.229591	–0.954756	–0.082137
C	4.737766	–0.976796	–3.661100
H	2.950389	–1.752182	–2.750484
C	6.037430	–0.515425	–3.447118
H	7.574719	–0.140787	–1.990810
H	4.321297	–0.982543	–4.661033
H	6.631315	–0.163665	–4.281625
C	4.439527	–1.820436	1.581804
C	4.130555	–0.849641	2.542041
C	5.536452	–2.674780	1.785298
C	4.915778	–0.727830	3.687362

H	3.278854	–0.197460	2.392771
C	6.318039	–2.542773	2.928382
H	5.765966	–3.443551	1.056273
C	6.008334	–1.569409	3.879387
H	4.669401	0.021386	4.429470
H	7.162765	–3.202946	3.081941
H	6.615251	–1.474137	4.771390
C	3.335975	–3.792430	–0.149882
C	3.860240	–4.449691	–1.269402
C	2.681001	–4.536439	0.845913
C	3.722504	–5.832829	–1.393808
H	4.377716	–3.887467	–2.036672
C	2.550147	–5.914483	0.714652
H	2.278364	–4.034823	1.718547
C	3.067578	–6.564458	–0.406909
H	4.133667	–6.335436	–2.260701
H	2.045881	–6.481856	1.487042
H	2.963520	–7.637825	–0.506547
C	–3.796307	–2.934526	1.581804
C	–5.084653	–3.457318	1.785298
C	–2.801089	–3.152345	2.542041
C	–5.361125	–4.200195	2.928382
H	–5.865185	–3.271697	1.056273
C	–3.088208	–3.893274	3.687362
H	–1.810432	–2.740840	2.392771
C	–4.363315	–4.418665	3.879387

H	–6.355215	–4.601663	3.081941
H	–2.316180	–4.054513	4.429470
H	–4.584266	–4.991907	4.771390
C	–3.489466	–3.190524	–1.289523
C	–3.215680	–2.728824	–2.588731
C	–3.737170	–4.551896	–1.080758
C	–3.214813	–3.614627	–3.661100
H	–2.992628	–1.679021	–2.750484
C	–3.719649	–5.436609	–2.159527
H	–3.941638	–4.917606	–0.082137
C	–3.465086	–4.970856	–3.447118
H	–3.011556	–3.251082	–4.661033
H	–3.909284	–6.489505	–1.990810
H	–3.457396	–5.661055	–4.281625
C	–4.952328	–0.992824	–0.149882
C	–5.269172	–0.053596	0.845913
C	–5.783666	–1.118220	–1.269402
C	–6.397166	0.748749	0.714652
H	–4.633441	0.044291	1.718547
C	–6.912631	–0.307369	–1.393808
H	–5.555503	–1.847479	–2.036672
C	–7.218777	0.625628	–0.406909
H	–6.636393	1.469143	1.487042
H	–7.553482	–0.412143	–2.260701
H	–8.096310	1.252429	–0.506547
C	–0.643220	4.754961	1.581804

C	–1.329467	4.001987	2.542041
C	–0.451798	6.132098	1.785298
C	–1.827570	4.621104	3.687362
H	–1.468421	2.938300	2.392771
C	–0.956913	6.742968	2.928382
H	0.099220	6.715248	1.056273
C	–1.645019	5.988075	3.879387
H	–2.353222	4.033127	4.429470
H	–0.807549	7.804609	3.081941
H	–2.030985	6.466045	4.771390
C	1.616353	4.785254	–0.149882
C	1.923426	5.567912	–1.269402
C	2.588171	4.590034	0.845913
C	3.190126	6.140198	–1.393808
H	1.177788	5.734947	–2.036672
C	3.847019	5.165733	0.714652
H	2.355077	3.990532	1.718547
C	4.151198	5.938830	–0.406909
H	3.419815	6.747579	–2.260701
H	4.590512	5.012713	1.487042
H	5.132791	6.385396	–0.506547
C	–1.018342	4.617229	–1.289523
C	–2.073472	5.512432	–1.080758
C	–0.755391	4.149273	–2.588731
C	–2.848417	5.939615	–2.159527
H	–2.287953	5.872362	–0.082137

C	–1.522952	4.591424	–3.661100
H	0.042240	3.431202	–2.750484
C	–2.572344	5.486280	–3.447118
H	–3.665434	6.630292	–1.990810
H	–1.309741	4.233625	–4.661033
H	–3.173919	5.824720	–4.281625

2. $[\{Pt(PPh_3)\}_3(\mu_3\text{-}S)(\mu\text{-}SMe)_3]^+$ (15a')

SCF energy E(RmPW+HF–PW91)	–5167.2451412 a.u.
Zero-point vibrational energies	608.04 kcal/mol
Sum of electronic and zero-point energies	–5166.276173 a.u.
Sum of electronic and thermal energies	–5166.208185 a.u.
Sum of electronic and thermal enthalpies	–5166.207240 a.u.
Sum of electronic and thermal free energies	–5166.390284 a.u.

	x	y	z
S	–2.619732	0.655248	0.940612
Pt	–0.499539	1.739016	1.035027
Pt	–1.256263	–1.302122	1.035027
Pt	1.755802	–0.436895	1.035027
P	–0.942650	3.508505	–0.334772
P	–2.567129	–2.570611	–0.334772
S	0.742405	–2.596379	0.940612
P	3.509779	–0.937893	–0.334772
S	1.877328	1.941131	0.940612
S	0.000000	0.000000	2.615208
C	–3.381862	0.876193	2.585144
H	–4.213886	0.172472	2.667789
H	–3.758181	1.900707	2.643915
H	–2.653899	0.697702	3.378316
C	2.449736	2.490682	2.585144
H	2.256308	3.563096	2.667789
H	3.525151	2.304327	2.643915
H	1.931177	1.949493	3.378316
C	0.932126	–3.366875	2.585144
H	1.957578	–3.735568	2.667789

H	0.233031	–4.205034	2.643915
H	0.722722	–2.647195	3.378316
C	–2.673933	4.073473	–0.333491
C	–3.067302	5.234198	0.344730
C	–3.642486	3.288422	–0.981109
C	–4.411775	5.601491	0.375966
H	–2.327006	5.852341	0.837324
C	–4.981391	3.664527	–0.946545
H	–3.350304	2.390398	–1.512003
C	–5.368090	4.819360	–0.266627
H	–4.708034	6.502915	0.898068
H	–5.722321	3.055526	–1.449404
H	–6.411307	5.109106	–0.241457
C	0.000000	4.976485	0.187150
C	0.096850	5.236926	1.564548
C	0.603652	5.849186	–0.724505
C	0.773152	6.366704	2.016388
H	–0.352738	4.548532	2.274149
C	1.288723	6.972312	–0.263430
H	0.546461	5.648289	–1.787097
C	1.370306	7.234683	1.101996
H	0.836543	6.568121	3.078903
H	1.758390	7.641961	–0.973300
H	1.900976	8.110370	1.454715
C	–0.560989	3.280446	–2.098517
C	–1.106530	4.140275	–3.065925

C	0.301254	2.251030	–2.497878
C	–0.775253	3.977517	–4.408431
H	–1.795845	4.921486	–2.766864
C	0.625162	2.089224	–3.844555
H	0.709810	1.571452	–1.758588
C	0.091329	2.955290	–4.797676
H	–1.196608	4.644419	–5.150609
H	1.283891	1.282420	–4.141866
H	0.346165	2.833237	–5.843495
C	–4.309762	–2.488242	0.187150
C	–5.367370	–2.401815	–0.724505
C	–4.583736	–2.534588	1.564548
C	–6.682561	–2.370089	–0.263430
H	–5.164793	–2.350896	–1.787097
C	–5.900303	–2.513783	2.016388
H	–3.762775	–2.579746	2.274149
C	–6.950572	–2.430621	1.101996
H	–7.497327	–2.298170	–0.973300
H	–6.106431	–2.559593	3.078903
H	–7.974275	–2.408892	1.454715
C	–2.190764	–4.352431	–0.333491
C	–1.026614	–4.798696	–0.981109
C	–2.999297	–5.273460	0.344730
C	–0.682878	–6.146274	–0.946545
H	–0.394994	–4.096648	–1.512003
C	–2.645146	–6.621455	0.375966

H	–3.904773	–4.941417	0.837324
C	–1.489643	–7.058583	–0.266627
H	0.214997	–6.483438	–1.449404
H	–3.277672	–7.328735	0.898068
H	–1.218962	–8.106908	–0.241457
C	–2.560455	–2.126054	–2.098517
C	–2.100077	–0.864621	–2.497878
C	–3.032318	–3.028421	–3.065925
C	–2.121902	–0.503205	–3.844555
H	–1.715822	–0.171013	–1.758588
C	–3.057005	–2.660147	–4.408431
H	–3.364210	–4.015990	–2.766864
C	–2.605021	–1.398552	–4.797676
H	–1.752554	0.470672	–4.141866
H	–3.423881	–3.358502	–5.150609
H	–2.626738	–1.116831	–5.843495
C	4.309762	–2.488242	0.187150
C	4.763717	–3.447371	–0.724505
C	4.486886	–2.702338	1.564548
C	5.393838	–4.602223	–0.263430
H	4.618332	–3.297394	–1.787097
C	5.127152	–3.852921	2.016388
H	4.115513	–1.968786	2.274149
C	5.580266	–4.804062	1.101996
H	5.738937	–5.343791	–0.973300
H	5.269888	–4.008528	3.078903

H	6.073299	–5.701478	1.454715
C	4.864698	0.278958	–0.333491
C	4.669100	1.510275	–0.981109
C	6.066599	0.039262	0.344730
C	5.664268	2.481748	–0.946545
H	3.745298	1.706249	–1.512003
C	7.056921	1.019964	0.375966
H	6.231779	–0.910924	0.837324
C	6.857734	2.239222	–0.266627
H	5.507323	3.427912	–1.449404
H	7.985707	0.825820	0.898068
H	7.630269	2.997802	–0.241457
C	3.121444	–1.154392	–2.098517
C	4.138848	–1.111854	–3.065925
C	1.798822	–1.386409	–2.497878
C	3.832257	–1.317370	–4.408431
H	5.160055	–0.905496	–2.766864
C	1.496739	–1.586018	–3.844555
H	1.006012	–1.400439	–1.758588
C	2.513692	–1.556738	–4.797676
H	4.620489	–1.285917	–5.150609
H	0.468663	–1.753092	–4.141866

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