

Supporting Information

Theoretical Study on the Stability of Osmasilbenzynes

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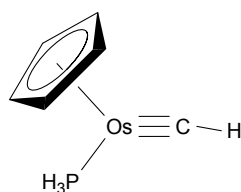
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Cartesian coordinates and electronic energies (in Hartree) for all the complexes calculated in this study

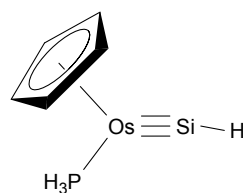
Osmium–Silicon Triple Bond



E: -331.558427

Os	0.139213	-0.318871	-0.000061
C	-2.064359	-0.605986	0.000374
C	-1.773146	0.184818	1.169339
C	-1.773579	0.184411	-1.168980
H	-2.478649	-1.605067	0.000625
C	-1.309837	1.451075	0.715660
H	-1.920310	-0.112439	2.197676
C	-1.310090	1.450807	-0.715937
H	-1.921100	-0.113228	-2.197155
H	-0.987003	2.264887	1.351009
H	-0.987358	2.264338	-1.351695

P	2.042971	0.959567	0.000026
H	2.995127	0.920231	1.068955
H	3.000231	0.912407	-1.063840
H	1.834939	2.370625	-0.005410
C	1.130564	-1.746806	0.000176
H	1.842052	-2.570959	0.000266

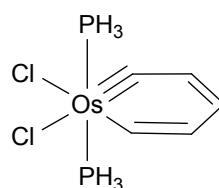


E: -297.354101

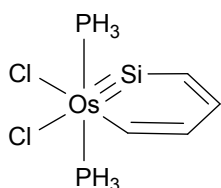
Os	0.089729	-0.143507	-0.000030
Si	1.692269	-1.587388	-0.000007
C	-1.945097	-1.066786	-0.000300
C	-1.845968	-0.232844	1.168951
C	-1.846057	-0.232149	-1.169069
H	-2.093969	-2.137379	-0.000613

C	-1.677458	1.109903	0.723177
H	-1.905676	-0.561207	2.196615
C	-1.677532	1.110321	-0.722498
H	-1.905800	-0.559919	-2.196919
H	-1.581677	1.978887	1.359477
H	-1.581664	1.979662	-1.358300
P	1.575156	1.606802	0.000006
H	2.500238	1.868615	1.063101
H	2.499373	1.869410	-1.063656
H	0.965072	2.901437	0.000719
H	2.918282	-2.442233	0.000276

H	0.595328	3.044360	-1.283718
Cl	2.235196	0.000601	-1.473917
Cl	1.624492	-0.001064	1.954846
H	-0.860735	-0.000822	2.366444
H	-3.149194	-0.001016	2.416013
Si	-1.596011	0.000576	-1.334920
H	-4.671541	-0.000396	0.629802



Structure Aspect of Osasilabenzynesilene



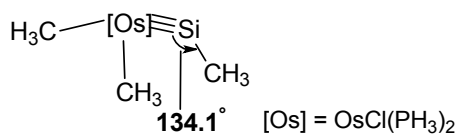
E: -296.366447

C	-3.341738	0.000386	-1.021010
C	-3.617059	-0.000212	0.342971
C	-2.691004	-0.000598	1.427326
C	-1.307354	-0.000479	1.369537
H	-4.147759	0.000648	-1.745681
Os	0.181858	0.000067	-0.056642
P	0.571596	-2.349228	-0.045939
P	0.571682	2.349328	-0.044207
H	1.840355	-2.702787	0.476533
H	-0.268431	-3.225603	0.701207
H	0.593515	-3.043814	-1.285744
H	-0.269262	3.225493	0.702165
H	1.839766	2.702601	0.480131

E: -330.583645

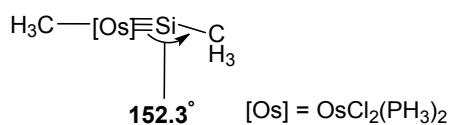
C	-3.425977	0.031970	-0.157515
C	-2.809612	-0.095086	1.110751
C	-1.435842	-0.120699	1.300800
Os	0.049064	0.009245	-0.082606
P	0.429148	-2.345037	-0.226329
P	0.465153	2.349077	0.167782
H	1.802311	-2.680888	-0.272144
H	-0.033631	-3.180036	0.826968
H	-0.066738	-3.066926	-1.349116
H	-0.269866	3.109201	1.122389
H	1.794948	2.638989	0.552896
H	0.315604	3.178213	-0.976417
Cl	1.547190	-0.250209	1.919195
H	-1.104703	-0.222360	2.335823
H	-3.467895	-0.175661	1.974056
H	-4.514057	0.040951	-0.207124
C	-1.350006	0.126685	-1.168604
C	-2.712779	0.147864	-1.355941

H -3.194210 0.243746 -2.323621
 Cl 2.099880 0.180042 -1.501807



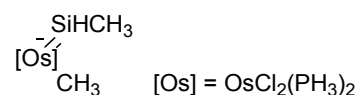
E: -221.375971

C -3.740577 -0.039124 -0.062803
 C -1.175058 -0.049357 1.836988
 H -4.566999 -0.028139 -0.779127
 Os 0.012211 -0.006218 -0.021813
 P 0.422481 -2.344405 0.010817
 P 0.270740 2.352426 -0.004336
 H 1.769744 -2.683048 0.294640
 H -0.244779 -3.186754 0.951369
 H 0.214146 -3.111224 -1.169389
 H -0.405140 3.143406 0.973862
 H 1.604746 2.778924 0.215217
 H -0.045603 3.111556 -1.165921
 Cl 1.675730 0.036269 -1.874895
 Cl 1.844956 0.075480 1.610329
 H -0.444034 -0.069566 2.647328
 Si -2.021282 -0.056774 -0.832744
 H -1.808063 0.834199 1.991213
 H -1.816277 -0.932756 1.954818
 H -3.809736 0.846243 0.580231
 H -3.834275 -0.924620 0.577234



E: -221.379625

C 3.902837 -0.029522 0.159486
 C 0.973702 -0.058909 -1.998686
 H 4.405142 0.856137 0.565425
 Os -0.001961 0.001297 -0.010657
 P -0.402343 -2.338604 0.060979
 P -0.356246 2.347258 -0.046955
 H -1.775516 -2.674582 0.150337
 H -0.010455 -3.162454 -1.037173
 H 0.115851 -3.126945 1.127762
 H 0.204137 3.156274 -1.082570
 H -1.721087 2.710490 -0.164996
 H 0.017747 3.131618 1.079734
 Cl -1.470840 0.078773 2.019685
 Cl -2.042701 -0.045683 -1.394780
 H 0.146638 -0.065580 -2.711961
 Si 2.072450 0.001767 0.559316
 H 1.601969 0.811892 -2.229347
 H 1.577904 -0.956750 -2.185595
 H 4.041884 -0.051211 -0.927801
 H 4.380300 -0.913946 0.597098

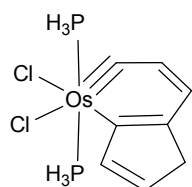


E: -222.087586

C 3.712633 -0.191365 -0.006377
 C -0.252173 -0.055679 -2.310469
 H 4.206635 -0.455164 0.939092
 Os -0.081903 -0.037313 -0.152844
 P -1.122048 -2.107508 -0.001934
 P 0.675308 2.156246 -0.180780
 H -2.227592 -2.240948 0.888546
 H -1.738771 -2.685435 -1.162751

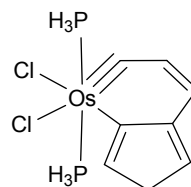
H	-0.410728	-3.285766	0.404571	Cl	-2.000367	-0.813120	1.622383
H	1.175509	2.757611	-1.388599	Cl	-1.933280	1.264904	-1.423395
H	-0.271177	3.173716	0.147709	H	0.704852	1.212479	-2.210539
H	1.734142	2.605513	0.672346	H	3.030297	1.261187	-2.251944
Cl	-0.297995	0.214184	2.435405	Si	1.534965	-1.008605	1.057430
Cl	-2.470292	0.906025	-0.228061	H	4.568503	0.268564	-0.802813
H	-1.235751	0.355189	-2.566422	H	1.545386	-2.008912	2.200175
Si	1.953067	-0.932967	-0.055328		[Os] = OsCl ₂ (PH ₃) ₂		
H	2.276743	-2.410514	0.050663	E:	-221.379626		
H	0.510930	0.555618	-2.816264	C	3.903341	-0.035198	0.159272
H	-0.185740	-1.061712	-2.751602	C	0.971205	-0.072951	-1.999505
H	3.712771	0.900097	-0.096005	H	4.406992	0.853233	0.557414
H	4.333990	-0.603200	-0.813635	Os	-0.001649	0.001497	-0.010609
				P	-0.407407	-2.337257	0.072616
[Os] = OsCl ₂ (PH ₃) ₂				P	-0.352265	2.347519	-0.060942
E:	-297.076780			H	-1.779472	-2.668658	0.190514
C	3.257384	-0.673547	0.588827	H	-0.040415	-3.160965	-1.033989
C	3.513837	0.118980	-0.524300	H	0.129853	-3.128727	1.127834
C	2.575239	0.732324	-1.409142	H	0.219273	3.152474	-1.093706
C	1.175457	0.707668	-1.343435	H	-1.715535	2.711551	-0.194534
H	4.120882	-1.097701	1.105630	H	0.010920	3.135186	1.066863
Os	-0.166401	0.008905	-0.033245	Cl	-1.468375	0.097214	2.020594
P	-0.938752	-1.880621	-1.198323	Cl	-2.044498	-0.056534	-1.391774
P	-0.075930	1.922194	1.322531	H	0.143244	-0.083205	-2.711703
H	-2.314284	-1.810206	-1.667235	Si	2.072924	0.002806	0.558211
H	-0.316074	-2.336649	-2.428719	H	1.600429	0.795404	-2.236654
H	-0.987785	-3.144735	-0.514826	H	1.573933	-0.972811	-2.181386
H	1.118327	2.756057	1.409406	H	4.042624	-0.066651	-0.927757
H	-1.031342	2.969570	1.036222	H	4.379229	-0.916523	0.604749
H	-0.321049	1.757573	2.729579				

The aromaticity of Osmasilabenzynes



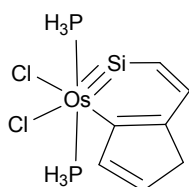
E: -446.101589

C	2.659925	-0.509166	0.057858
C	1.548889	0.365458	-0.099374
C	1.372039	-2.579404	0.481567
C	2.587267	-1.876508	0.328152
H	1.328632	-3.642362	0.693040
H	3.515616	-2.438902	0.425693
C	2.112854	1.688049	-0.380356
C	3.466474	1.645833	-0.394598
C	3.954548	0.257265	-0.119001
H	1.500341	2.563611	-0.547878
H	4.595121	0.220245	0.775659
Os	-0.438417	-0.165645	0.038756
P	-0.656027	0.520758	2.310000
H	-1.952580	0.981153	2.645742
H	-0.427678	-0.415143	3.360753
H	0.150019	1.598687	2.766554
P	-0.831548	-0.449693	-2.298474
H	-1.333225	-1.704450	-2.736990
H	-1.805826	0.436245	-2.816956
H	0.221856	-0.266887	-3.242526
Cl	-1.027395	2.258887	-0.337568
Cl	-2.900915	-0.583924	0.093223
C	0.285871	-1.764773	0.331871
H	4.127600	2.487230	-0.577438
H	4.567472	-0.131253	-0.946842



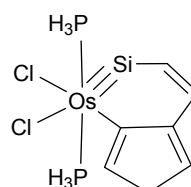
E: -446.081892

C	2.708206	-0.528640	-0.000442
C	1.561204	0.442373	-0.000233
C	1.391499	-2.623323	-0.001209
C	2.597152	-1.964541	-0.000862
H	1.306820	-3.705881	-0.001578
H	3.518543	-2.545136	-0.000928
C	2.117906	1.679039	0.000028
C	3.625413	1.608483	-0.000098
C	3.899107	0.139495	-0.000338
H	1.575211	2.615200	0.000380
H	4.077314	2.102462	-0.876052
H	4.888292	-0.307343	-0.000471
H	4.077390	2.102214	0.875953
Os	-0.470120	-0.186022	-0.000182
P	-0.684360	0.098932	2.361472
H	0.245619	0.953533	3.015761
H	-1.917704	0.665496	2.764713
H	-0.623961	-1.034269	3.223219
P	-0.686235	0.102121	-2.361366
H	-1.920132	0.668894	-2.762622
H	0.242866	0.957771	-3.015565
H	-0.626394	-1.029963	-3.224584
Cl	-1.053314	2.256937	0.002410
Cl	-2.925084	-0.623545	-0.000069
C	0.279008	-1.767682	-0.001142



E: -411.877854

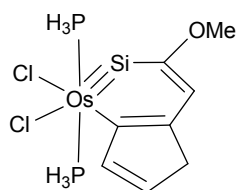
C	-2.742975	-0.163904	0.020616
C	-1.497483	0.522825	-0.032906
C	-2.153262	-2.631000	-0.173080
C	-3.026582	-1.543175	-0.024020
H	-2.538654	-3.641849	-0.221690
H	-4.089264	-1.793663	0.038563
C	-1.856495	1.951455	-0.096283
C	-3.194450	2.139651	-0.046019
C	-3.893712	0.827310	0.052991
H	-1.119612	2.739142	-0.156824
H	-4.604960	0.675401	-0.773746
Os	0.500581	-0.128167	-0.033765
P	0.926069	0.428800	-2.304892
H	1.784162	1.547798	-2.461388
H	1.590936	-0.523320	-3.123134
H	-0.129741	0.803510	-3.189235
P	0.681842	-0.285590	2.334402
H	0.481845	-1.511652	3.035474
H	1.964152	0.069655	2.822107
H	-0.150811	0.560036	3.117296
Cl	1.166583	2.200002	0.560016
Cl	2.948500	-0.612454	-0.092154
H	-3.705052	3.097221	-0.069163
H	-4.484738	0.747062	0.979275
Si	-0.494838	-2.056004	-0.288250



E: -411.861551

C	2.831957	-0.182244	0.031861
C	1.518095	0.570149	-0.028962
Si	0.490846	-2.034825	-0.242216
C	2.188902	-2.624001	-0.121305
C	3.093684	-1.605217	0.015002
H	2.520976	-3.656399	-0.152140
H	4.150478	-1.870660	0.095615
C	1.878878	1.881094	-0.087076
C	3.369784	2.081113	-0.038703
C	3.885115	0.687302	0.044055
H	1.195630	2.717466	-0.127635
H	3.764532	2.603314	-0.925812
H	4.934652	0.412523	0.081446
H	3.687954	2.689754	0.823554
Os	-0.543887	-0.140283	-0.027056
P	-0.680769	-0.183082	2.343834
H	-1.952658	0.180234	2.856202
H	-0.449360	-1.365509	3.110180
H	0.162518	0.713548	3.056352
P	-0.837125	0.389908	-2.323579
H	-1.535275	-0.518258	-3.166085
H	-1.600513	1.567039	-2.541932
H	0.286229	0.673219	-3.156345
Cl	-1.168274	2.201107	0.470489
Cl	-2.980648	-0.609860	-0.099851

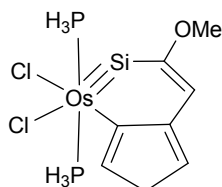
Effect of the Substituents on the Stabilization for Osmasilabenyne



E: -526.386519

C	-2.070389	1.394378	0.067410
C	-0.663472	1.353096	-0.020181
C	-2.846831	-1.016644	-0.098815
C	-3.038028	0.352573	0.061631
C	-0.243326	2.765403	-0.117022
C	-1.294850	3.611480	-0.055457
C	-2.559589	2.833182	0.087821
H	0.790567	3.065352	-0.208091
H	-3.269837	3.045397	-0.726561
Os	0.728409	-0.236813	-0.038663
P	1.383363	0.091383	-2.299444
H	2.688258	0.631210	-2.438909
H	1.484903	-1.046671	-3.143896
H	0.661964	0.967038	-3.164925
P	0.779411	-0.518358	2.323205
H	0.029309	-1.535402	2.984309
H	2.073741	-0.803921	2.824145
H	0.413862	0.592999	3.131324
Cl	2.453048	1.427183	0.615259
H	-1.250371	4.694868	-0.096259
H	-3.088471	3.076305	1.023346
Si	-1.109981	-1.389593	-0.310183
Cl	2.597013	-1.886025	-0.119301
H	-4.069267	0.694676	0.164845

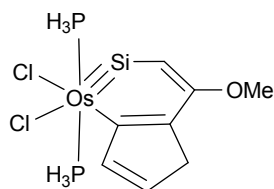
O	-3.825697	-1.976119	-0.129356
C	-5.177768	-1.549649	-0.048019
H	-5.439625	-0.878751	-0.877768
H	-5.780247	-2.457380	-0.111928
H	-5.385660	-1.042652	0.904228



E: -526.375734

C	2.167774	1.433374	0.088872
C	0.657128	1.399324	-0.020961
Si	1.096974	-1.353084	-0.338384
C	2.869672	-0.982012	-0.116592
C	3.128430	0.344471	0.086840
H	4.163227	0.659429	0.222452
C	0.286273	2.705329	-0.105172
C	1.453956	3.649314	-0.012611
C	2.613133	2.722090	0.119153
H	-0.730590	3.064931	-0.176085
H	1.552644	4.296506	-0.899675
H	3.650730	3.033528	0.186632
H	1.366551	4.336475	0.844734
Os	-0.755469	-0.259444	-0.040597
P	-0.769214	-0.505020	2.322913
H	-2.042044	-0.826634	2.859110
H	0.024461	-1.478688	3.001792
H	-0.430325	0.639526	3.095902
P	-1.335358	0.187281	-2.302239
H	-1.548841	-0.899636	-3.193976

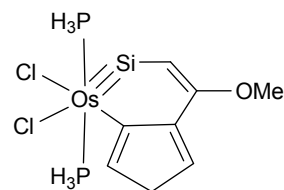
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H	-0.500411	1.010660	-3.113638
Cl	-2.440516	1.412522	0.634825
Cl	-2.621581	-1.888620	-0.141550
O	3.778279	-1.999964	-0.173774
C	5.154360	-1.668806	-0.022883
H	5.351115	-1.219392	0.959343
H	5.698405	-2.610508	-0.108538
H	5.486061	-0.978904	-0.809963



E: -526.406278

C	2.301383	0.742797	0.045626
C	0.917900	1.004785	-0.003857
C	2.446645	-1.752447	-0.366314
C	3.005814	-0.495837	-0.073086
C	0.811644	2.480273	-0.016926
C	2.022047	3.071004	0.063130
C	3.091830	2.034163	0.133788
H	-0.134186	2.999404	-0.065425
H	3.673773	2.102027	1.065189
Os	-0.835129	-0.197336	-0.056288
P	-0.825827	-0.681792	2.271851
H	-2.121642	-0.753083	2.842471
H	-0.262835	-1.881889	2.800227
H	-0.201186	0.256361	3.138758
P	-1.471291	0.491974	-2.237479
H	-1.938465	-0.492790	-3.149420

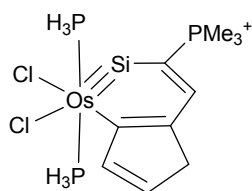
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H	-0.571333	1.196309	-3.092590
Cl	-2.066927	1.756286	0.857212
H	2.214501	4.139034	0.080623
H	3.824879	2.134623	-0.679653
Si	0.699519	-1.679455	-0.521661
Cl	-3.041390	-1.342652	-0.143543
H	3.065184	-2.631793	-0.483441
O	4.344757	-0.339616	0.084108
C	5.214739	-1.457084	-0.059928
H	5.148503	-1.886694	-1.066265
H	6.220172	-1.066768	0.104391
H	4.996505	-2.230479	0.685521



E: -526.391211

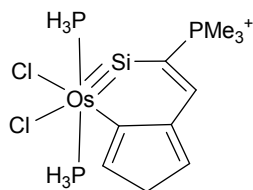
C	2.392747	0.786703	0.046692
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Si	0.704498	-1.602319	-0.618027
C	2.481890	-1.681212	-0.477562
C	3.085989	-0.498292	-0.100189
C	0.817348	2.430610	0.026315
C	2.159701	3.096021	0.130441
C	3.103188	1.943918	0.140313
H	-0.101844	2.999104	0.032697
H	2.373043	3.778379	-0.708705
H	4.181867	2.027019	0.172474
H	2.252504	3.712300	1.039629

Os	-0.868260	-0.211887	-0.059241	H	2.215751	2.732483	-0.537589
P	-0.788389	-0.738927	2.252327	H	-1.661914	4.106063	-0.548430
H	-2.062556	-0.866698	2.863166	Os	1.131485	-0.321107	-0.037212
H	-0.172215	-1.926195	2.753524	P	1.894584	-0.321066	-2.312218
H	-0.173578	0.208815	3.116852	H	3.306449	-0.252293	-2.408257
P	-1.468689	0.609244	-2.203393	H	1.614710	-1.467232	-3.099690
H	-1.967824	-0.291626	-3.184514	H	1.513249	0.714283	-3.214144
H	-2.528747	1.554780	-2.179995	P	1.149787	-0.561994	2.351911
H	-0.526257	1.329501	-2.996001	H	0.151717	-1.311288	3.039150
Cl	-2.075859	1.701939	0.924911	H	2.324764	-1.203078	2.810053
Cl	-3.053282	-1.377359	-0.164414	H	1.141031	0.626106	3.130251
H	3.062264	-2.581753	-0.636749	Cl	3.258364	0.762854	0.565273
O	4.410544	-0.397298	0.128323	H	0.851808	4.930850	-0.277377
C	5.245378	-1.541630	-0.034974	H	-1.233837	4.028722	1.156401
H	6.253291	-1.204308	0.209088	Si	-0.982579	-0.869458	-0.246506
H	4.949634	-2.345290	0.648757	Cl	2.363788	-2.448062	-0.039729
H	5.218139	-1.906176	-1.068169	P	-4.145168	-0.550364	-0.056175



E: -537.333266

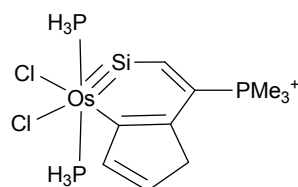
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C	0.335553	1.592587	-0.081338	H	-3.609354	-2.883574	0.401234
C	-2.481462	0.058786	-0.032383	H	-5.192459	-2.710716	-0.393354
C	-2.216038	1.457309	0.157729	C	-5.012786	-0.267588	1.540683
H	-3.081918	2.108478	0.307281	H	-5.026753	0.802333	1.767905
C	1.160500	2.778919	-0.312937	H	-6.042342	-0.633673	1.481855
C	0.453411	3.926873	-0.171926	H	-4.481870	-0.791710	2.339945
C	-0.967114	3.636127	0.162808	C	-5.161441	0.258388	-1.358347
				H	-6.183706	-0.131186	-1.335627
				H	-5.188192	1.338571	-1.188366
				H	-4.715958	0.065419	-2.337986



E: -537.304597

C	-1.036450	2.188222	-0.161772
C	0.359206	1.666110	0.046014
Si	-0.965893	-0.832607	0.350519
C	-2.492419	0.149764	0.033005
C	-2.288690	1.497004	-0.205033
C	1.115811	2.784912	0.215762
C	0.324551	4.057002	0.080894
C	-1.050294	3.563426	-0.174609
H	2.185139	2.804412	0.372517
H	0.353972	4.695728	0.979077
H	-1.924867	4.192973	-0.305473
H	0.686878	4.700148	-0.738049
Os	1.150894	-0.360435	0.042974
P	1.076868	-0.621366	-2.332854
H	2.199252	-1.316618	-2.846431
H	0.026977	-1.323928	-2.996581
H	1.095132	0.566377	-3.112246
P	1.917814	-0.133269	2.301454
H	1.731370	-1.219903	3.196483
H	3.321675	0.046570	2.393188
H	1.463073	0.951319	3.104692
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H	-3.148935	2.140389	-0.400249
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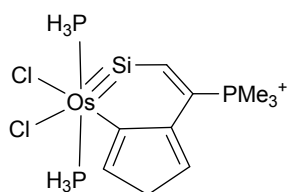
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C	-4.509622	-1.275342	1.711243
H	-4.467992	-0.487064	2.467956
H	-5.505835	-1.727974	1.707540
H	-3.769205	-2.043793	1.953697
C	-5.433365	0.680568	-0.320697
H	-5.273384	1.102427	-1.316637
H	-6.410295	0.188698	-0.296498
H	-5.421338	1.480757	0.424252



E: -537.310439

C	-1.724832	0.835048	0.081529
C	-0.299152	1.038580	-0.010863
C	-1.914231	-1.600560	-0.588054
C	-2.432056	-0.365513	-0.149924
C	-0.126132	2.499830	-0.006584
C	-1.291739	3.152384	0.175676
C	-2.410976	2.177026	0.323680
H	0.836974	2.978389	-0.105009
H	-3.228364	2.404734	-0.376157
Os	1.370496	-0.195579	-0.082162
P	2.254690	0.705831	-2.121972
H	3.412041	1.496300	-1.912251
H	2.717044	-0.219524	-3.092000
H	1.481004	1.579657	-2.940684

P	1.311945	-1.010078	2.174978	Si	0.085546	-1.333909	-1.217327
H	0.902009	-2.341691	2.468063	C	1.917728	-1.358713	-0.962822
H	2.590381	-0.982712	2.779095	C	2.495867	-0.281349	-0.359687
H	0.528317	-0.298457	3.124261	C	0.125701	2.478247	0.220588
Cl	2.525925	1.609956	1.141930	C	1.418685	3.216002	0.385328
H	-1.426054	4.226756	0.239256	C	2.429242	2.135268	0.237545
H	-2.830485	2.251293	1.337930	H	-0.824357	2.983435	0.331396
Si	-0.147985	-1.623158	-0.759102	H	1.570861	4.007734	-0.366006
Cl	3.531093	-1.366151	-0.151768	H	3.495265	2.328408	0.247926
H	-2.553498	-2.448602	-0.792114	H	1.490403	3.722023	1.361664
P	-4.284575	-0.371157	-0.031147	Os	-1.422069	-0.203176	-0.106663
C	-4.902497	-2.096061	0.099963	P	-1.059674	-1.420585	1.915435
H	-4.419069	-2.607681	0.936115	H	-2.259826	-1.667362	2.625600
H	-5.981411	-2.056325	0.276958	H	-0.492179	-2.729576	1.925223
H	-4.722222	-2.650674	-0.823280	H	-0.260243	-0.810976	2.921389
C	-4.965803	0.494354	1.442657	P	-2.424620	1.152601	-1.818717
H	-4.940538	1.576353	1.313328	H	-3.033410	0.486444	-2.914092
H	-6.004313	0.177260	1.577515	H	-3.508594	1.935741	-1.345650
H	-4.388190	0.219166	2.329271	H	-1.661391	2.146701	-2.495915
C	-5.044564	0.339053	-1.546596	Cl	-2.365878	1.277662	1.582138
H	-6.132949	0.239860	-1.490070	Cl	-3.552977	-1.384975	-0.237007
H	-4.782019	1.393918	-1.650719	H	2.503026	-2.225113	-1.255041
H	-4.672868	-0.208302	-2.417333	P	4.313640	-0.410939	-0.021273

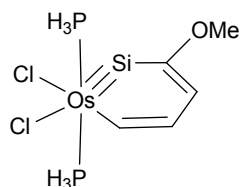


E: -537.289532

C	1.791256	0.946841	0.003877
C	0.290116	1.140420	0.027437

H	4.795390	-2.428065	-1.320702
H	5.934924	-2.191467	0.021510
H	4.303270	-2.824365	0.351990
C	5.317281	0.621516	-1.164734
H	5.107343	1.683178	-1.027940
H	6.378930	0.432199	-0.977848
H	5.075488	0.341718	-2.194216

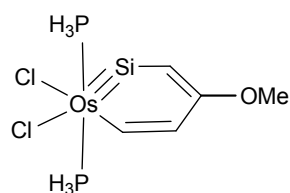
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H	5.769167	-0.067629	1.890400
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H	4.167790	-0.686738	2.378471



E: -410.877030

C	-3.073290	0.002385	-0.220138
C	-3.055093	-0.043550	1.160464
C	-1.898794	-0.071312	2.017161
C	-0.567035	-0.058120	1.678779
Os	0.593634	0.001972	-0.044890
P	0.976408	-2.344455	-0.163410
P	0.949786	2.353917	-0.021340
H	2.335536	-2.698912	0.021685
H	0.349857	-3.227576	0.763319
H	0.689573	-3.031956	-1.374359
H	0.255800	3.187344	0.903657
H	2.289913	2.713460	0.267022
H	0.730861	3.092224	-1.216048
Cl	2.304053	0.067276	-1.856146
Cl	2.419656	-0.049581	1.618242
H	0.081133	-0.087180	2.555926
H	-2.143315	-0.107405	3.078893
Si	-1.411616	0.024774	-0.921721
H	-4.013835	-0.061283	1.679914
O	-4.180759	0.028991	-1.026447
C	-5.455367	0.009618	-0.398454

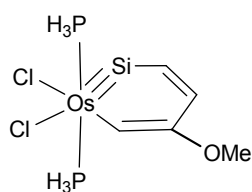
H	-6.186845	0.037695	-1.207712
H	-5.598601	-0.905523	0.191924
H	-5.596078	0.883618	0.251815



E: -410.898572

C	-2.870217	0.000084	-1.109728
C	-3.217844	-0.000867	0.244167
C	-2.294047	-0.001836	1.352407
C	-0.923054	-0.001800	1.315508
H	-3.622643	0.000558	-1.887747
Os	0.637593	0.000044	-0.068286
P	0.996383	-2.350655	-0.038082
P	0.992874	2.351084	-0.034567
H	2.229060	-2.727603	0.552225
H	0.106768	-3.219947	0.659486
H	1.078867	-3.047786	-1.274517
H	0.099550	3.218646	0.660432
H	2.222882	2.729372	0.560515
H	1.078871	3.049095	-1.270237
Cl	2.731028	0.002592	-1.415292
Cl	1.988946	-0.001303	1.996564
H	-0.499295	-0.002637	2.321808
H	-2.794203	-0.002638	2.319585
Si	-1.122984	0.000196	-1.370658
O	-4.499016	-0.001055	0.668581
C	-5.559910	0.000268	-0.282551
H	-6.479366	0.000671	0.304067
H	-5.525086	0.896490	-0.912555

H -5.526547 -0.895341 -0.913501



E: -410.878157

C 2.342472 -2.256000 -0.148628

C 3.117517 -1.096116 -0.074974

C 2.660207 0.248183 0.008720

C 1.338757 0.678065 0.035441

Os -0.569438 -0.085792 -0.005688

P -0.942761 0.229400 -2.336410

P -0.910275 -0.085400 2.350050

H -1.964811 1.170670 -2.611510

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H 0.162396 0.203652 3.242912

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H -1.421981 -1.260624 2.963362

Cl -2.995440 -0.640166 -0.020494

Cl -1.154357 2.315376 0.140719

H 1.310649 1.767977 0.101811

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O 3.579263 1.293652 0.072619

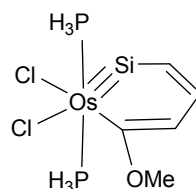
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H 5.457905 1.993249 0.132063

H 2.833010 -3.220778 -0.209664



E: -410.886129

C -2.311721 -2.406454 -0.797665

C -3.088716 -1.464749 -0.097732

C -2.787334 -0.148884 0.296251

C -1.567569 0.549804 0.133758

Os 0.385409 -0.118339 -0.104332

P 0.510606 -1.293840 1.961678

P 0.799311 1.369188 -1.911524

H 1.744804 -1.111162 2.632510

H -0.411473 -0.940899 2.984999

H 0.395897 -2.713606 2.037354

H -0.274256 2.015088 -2.592247

H 1.573297 2.503063 -1.550188

H 1.543865 0.896169 -3.025292

Cl 2.817394 -0.580716 -0.325314

Cl 0.975065 1.692017 1.470226

Si -0.669652 -1.819861 -1.027742

H -4.113331 -1.772889 0.125234

H -2.751428 -3.347952 -1.103233

O -1.629042 1.897369 0.168577

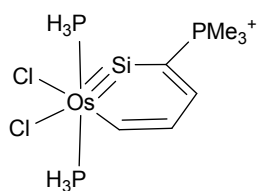
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H -3.260233 2.446137 1.358628

H -2.579547 3.668735 0.254694

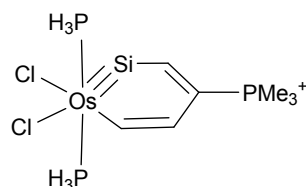
H -3.639778 0.401971 0.680844



E: -421.815944

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C	2.238937	-0.003162	1.754993
C	0.999328	-0.004281	2.400052
C	-0.282133	-0.003171	1.818443
Os	-1.142405	0.000036	-0.018422
P	-1.587324	2.361153	-0.169977
P	-1.587709	-2.360485	-0.177997
H	-2.975043	2.633688	-0.195042
H	-1.143175	3.239528	0.857824
H	-1.134557	3.054731	-1.322555
H	-1.144362	-3.242274	0.847217
H	-2.975467	-2.632622	-0.204824
H	-1.134387	-3.050435	-1.332537
Cl	-2.512551	0.003642	-2.061048
Cl	-3.181523	-0.002243	1.340912
H	-1.050941	-0.004719	2.594260
H	1.046119	-0.006238	3.487491
Si	0.973615	0.000968	-0.609846
H	3.105053	-0.004325	2.422245
P	4.152359	0.000445	-0.260430
C	4.153674	0.002899	-2.092895
H	3.648767	-0.890377	-2.471915
H	3.646788	0.896036	-2.469597
H	5.186831	0.004529	-2.452518
C	5.088159	1.477930	0.304059
H	5.114623	1.503386	1.397288

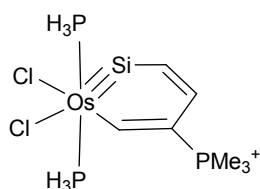
H	6.113211	1.440953	-0.077196
H	4.593613	2.382866	-0.059181
C	5.088698	-1.478273	0.299936
H	6.113262	-1.440589	-0.082561
H	5.116600	-1.505989	1.393074
H	4.593608	-2.382407	-0.064554



E: -421.806787

C	2.118528	-0.003938	-1.496112
C	2.582088	-0.000775	-0.184250
C	1.812375	0.003006	1.013091
C	0.421635	0.003549	1.125288
Os	-1.232698	-0.000001	-0.067061
P	-1.713277	2.354163	-0.012091
P	-1.710941	-2.354397	-0.003789
H	-2.922391	2.631401	0.667707
H	-0.818154	3.258805	0.626742
H	-1.914437	3.016529	-1.250653
H	-0.815144	-3.255832	0.638625
H	-2.920037	-2.630312	0.676564
H	-1.911009	-3.021457	-1.240009
Cl	-3.437633	-0.003133	-1.165995
Cl	-2.346836	0.003175	2.123304
H	0.123764	0.006633	2.175941
H	2.369794	0.005663	1.950541
Si	0.327290	-0.003068	-1.610519
H	2.792859	-0.006649	-2.344292
P	4.403646	0.000505	0.094521

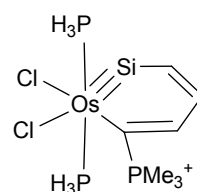
C	4.893102	-1.482360	1.056639	Cl	-1.066632	-2.376309	0.000046
H	5.972800	-1.467989	1.233671	H	1.111782	-1.305921	-0.000223
H	4.368199	-1.493353	2.015062	Si	-0.362673	2.162833	-0.000054
H	4.626792	-2.381620	0.494256	H	1.528973	3.930693	-0.000031
C	5.323778	-0.017096	-1.488240	H	3.310796	2.325266	-0.000132
H	5.080648	0.870871	-2.077823	P	3.707997	-0.422641	-0.000010
H	6.396275	-0.017614	-1.271781	C	3.443770	-2.234714	-0.002130
H	5.075835	-0.915653	-2.059493	H	2.889424	-2.542990	0.887739
C	4.893897	1.501972	1.026816	H	2.890073	-2.540888	-0.893131
H	5.972274	1.487310	1.211607	H	4.423277	-2.722705	-0.002327
H	4.634975	2.389663	0.443022	C	4.721447	-0.018752	1.480111
H	4.362070	1.535682	1.980975	H	5.669418	-0.564232	1.446640



E: -421.820522

C	1.282744	2.874493	-0.000071
C	2.289226	1.935707	-0.000147
C	2.139496	0.499611	-0.000239
C	0.948807	-0.228406	-0.000176
Os	-1.066703	0.092059	-0.000019
P	-1.485180	-0.152421	2.353883
P	-1.485520	-0.152505	-2.353849
H	-2.228795	-1.321930	2.638500
H	-0.411390	-0.273160	3.282747
H	-2.261447	0.851866	2.986288
H	-0.411868	-0.273224	-3.282874
H	-2.229136	-1.322049	-2.638321
H	-2.261927	0.851738	-2.986151
Cl	-3.527826	0.065574	0.000179

H	4.929995	1.054163	1.513114
H	4.170582	-0.300176	2.381926
C	4.723703	-0.015772	-1.477773
H	4.932483	1.057165	-1.508354
H	5.671560	-0.561425	-1.443881
H	4.174220	-0.295367	-2.380997

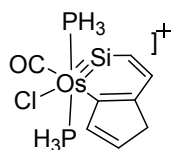


E: -421.811447

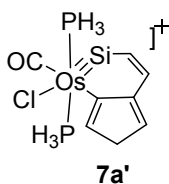
C	-0.161598	3.626317	-0.241375
C	1.161910	3.297035	-0.043819
C	1.796684	2.000198	0.042626
C	1.259230	0.718680	0.011878
Os	-0.742940	0.014329	-0.031144
P	-1.177868	0.044691	2.330874
P	-0.912509	-0.674061	-2.327502
H	-1.370992	-1.253152	2.862877

H	-0.233395	0.585840	3.251036	E:	-510.024027		
H	-2.355402	0.707946	2.760580	C	-2.730793	-0.173571	-0.000016
H	0.074599	-0.344562	-3.302795	C	-1.489739	0.505764	-0.000020
H	-0.977555	-2.081708	-2.479168	C	-2.148866	-2.664994	-0.000171
H	-2.085539	-0.263418	-3.008755	C	-3.019401	-1.559057	-0.000076
Cl	-2.989653	-0.999975	-0.022106	H	-2.528323	-3.678228	-0.000225
Cl	0.051072	-2.284374	0.442530	H	-4.082634	-1.809228	-0.000071
Si	-1.123304	2.135127	-0.302177	C	-1.806250	1.929068	0.000035
H	1.862549	4.130557	0.034587	C	-3.150494	2.134257	0.000043
H	-0.478645	4.659133	-0.321858	C	-3.865641	0.831438	0.000021
H	2.870281	2.126051	0.124243	H	-1.056518	2.708744	0.000058
P	2.711338	-0.487403	0.031186	H	-4.521677	0.724139	-0.877652
C	2.959008	-1.334368	1.647039	Os	0.609013	-0.172161	-0.000027
H	3.857193	-1.956467	1.579592	P	0.642255	0.242037	-2.375166
H	3.113586	-0.567921	2.412808	H	1.879676	0.703267	-2.890412
H	2.095089	-1.948835	1.892160	H	0.322029	-0.768036	-3.323334
C	4.338783	0.360554	-0.221503	H	-0.231468	1.279852	-2.785230
H	5.100095	-0.423202	-0.289071	P	0.641982	0.241534	2.375204
H	4.346027	0.935970	-1.150345	H	0.321426	-0.768675	3.323117
H	4.594646	1.011228	0.617906	H	1.879401	0.702439	2.890747
C	2.694220	-1.671480	-1.376691	H	-0.231626	1.279420	2.785329
H	2.724109	-1.098564	-2.308633	H	-3.648307	3.098069	0.000074
H	3.594611	-2.290663	-1.315147	H	-4.521640	0.724096	0.877718
H	1.810492	-2.305079	-1.337079	Si	-0.517501	-2.051481	-0.000227
				C	2.498765	-0.711111	0.000021
				O	3.590526	-1.059567	0.000061
				Cl	1.392144	2.181252	0.000294

**Effect of the Ligand on the
Stabilization for Osmasilabenzyne**



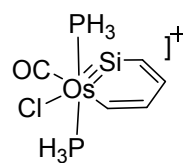
7a



7a'

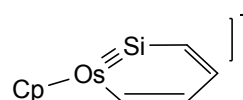
E: -510.015767

C	-2.866453	-0.166534	-0.054517
C	-1.519470	0.512875	0.013447
Si	-0.600990	-1.951283	-0.049471
C	-2.248970	-2.603402	-0.130137
C	-3.166867	-1.573046	-0.124544
H	-2.554438	-3.642173	-0.177794
H	-4.225531	-1.832295	-0.171355
C	-1.789660	1.841906	0.091633
C	-3.268368	2.124876	0.070191
C	-3.866095	0.766965	-0.026519
H	-1.052390	2.632275	0.150541
H	-3.613915	2.660231	0.969006
H	-4.930167	0.558521	-0.063341
H	-3.565472	2.765278	-0.775706
Os	0.653147	-0.177299	0.010985
P	0.712032	0.260882	-2.363276
H	1.950813	0.728337	-2.868841
H	0.401955	-0.740468	-3.326470
H	-0.169511	1.297088	-2.758949
P	0.559194	0.137309	2.402171
H	1.542976	-0.462349	3.235565
H	0.674469	1.500067	2.776894
H	-0.617937	-0.244161	3.098818
C	2.524922	-0.703272	0.047501
O	3.615147	-1.060153	0.075847
Cl	1.420590	2.169321	-0.043714



E: -394.501949

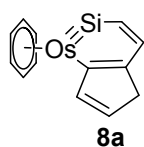
C	-2.690687	0.000082	1.403827
C	-1.325369	0.000094	1.329704
C	-3.346159	-0.000108	-1.052679
C	-3.629741	-0.000014	0.303908
H	-4.132520	-0.000193	-1.797678
H	-4.684883	-0.000040	0.582855
Os	0.270056	0.000010	-0.147348
P	0.509489	2.377737	0.220008
H	1.850477	2.834825	0.231356
H	-0.096524	3.335897	-0.637425
H	0.050703	2.813025	1.487698
P	0.509469	-2.377660	0.220332
H	-0.096818	-3.335941	-0.636774
H	1.850421	-2.834862	0.231431
H	0.050961	-2.812662	1.488219
Si	-1.593917	-0.000086	-1.284043
C	1.787684	-0.000128	-1.401875
O	2.630705	-0.000312	-2.177733
Cl	1.757603	0.000112	1.814653
H	-0.833110	0.000179	2.305683
H	-3.151733	0.000136	2.390040



E: -443.279232

C	3.338116	-0.831788	0.000141
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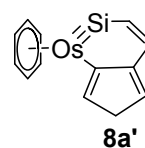
C	3.532664	0.551890	0.000149
C	2.509640	1.530354	0.000028
C	1.119213	1.326145	-0.000098
H	4.193931	-1.502138	0.000263
Os	-0.293866	-0.138185	-0.000145
H	0.611299	2.304938	-0.000116
H	2.860568	2.567389	-0.000003
Si	1.595351	-1.231425	-0.000018
H	4.562511	0.925877	0.000158
C	-2.448957	-0.950876	0.000816
C	-2.221076	-0.146098	1.165651
C	-2.221914	-0.146943	-1.164802
H	-2.655166	-2.013457	0.001300
C	-1.924097	1.192375	0.719528
H	-2.324675	-0.465891	2.193575
C	-1.924492	1.191887	-0.719809
H	-2.326436	-0.467313	-2.192450
H	-1.737948	2.045847	1.358109
H	-1.739796	2.045075	-1.359188



E: -597.462459

C	2.695197	0.058517	0.004856
C	1.362637	0.561199	-0.003699
C	2.390457	-2.437293	0.005782
C	3.162477	-1.273845	0.009940
H	2.849873	-3.417768	0.008282
H	4.248077	-1.397236	0.016415
C	1.537083	2.037352	-0.010088

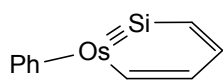
C	2.829649	2.414102	-0.004747
C	3.699937	1.200094	0.005875
H	0.710498	2.737234	-0.019425
H	4.357042	1.173322	0.889661
Os	-0.584336	-0.212152	-0.004271
H	3.204127	3.432832	-0.008116
H	4.367943	1.165980	-0.869383
Si	0.694656	-1.954781	-0.013598
C	-2.161709	0.571066	-1.422785
C	-2.744276	-0.501834	0.724817
C	-1.636921	1.687831	-0.707421
C	-2.129969	0.568201	1.444122
C	-1.620164	1.685523	0.717851
C	-2.760020	-0.500160	-0.691844
H	-2.142964	0.555142	-2.505516
H	-1.179546	2.503353	-1.254585
H	-1.148979	2.499019	1.256229
H	-2.087322	0.551593	2.526128
H	-3.107039	-1.369913	1.262467
H	-3.133602	-1.367587	-1.223121



E: -597.442473

C	2.709823	0.043338	0.251890
C	1.371415	0.619129	-0.155043
C	2.217983	-2.408647	0.222381
C	3.025765	-1.354157	0.508981
H	2.584606	-3.422661	0.358822
H	4.032879	-1.541754	0.887788

C	1.616678	1.933214	-0.431344	H	-3.043153	2.475075	-0.000113
C	3.056354	2.306992	-0.203745	Si	-1.627123	-1.204187	-0.002518
C	3.660131	1.016751	0.249286	H	-4.673924	0.755954	0.004537
H	0.885308	2.656642	-0.773733	C	2.229577	-1.048521	-0.691028
Os	-0.597060	-0.192470	-0.165837	C	1.959391	0.142551	-1.431023
H	3.167621	3.110517	0.543110	C	2.222073	-1.033460	0.725575
Si	0.632577	-1.949791	-0.588248	H	2.330802	-1.992150	-1.214351
C	-2.819765	0.042827	-0.654798	C	1.777660	1.387585	0.700422
C	-1.873699	-0.218276	1.594654	H	1.924909	0.121676	-2.513283
C	-2.346749	1.398495	-0.731257	C	1.946659	0.174161	1.436453
C	-1.285729	1.088941	1.464380	H	2.319036	-1.965257	1.270410
C	-1.614509	1.921938	0.340155	H	1.549603	2.307345	1.227265
C	-2.710524	-0.704501	0.545647	H	1.902785	0.177919	2.518556
H	-3.330168	-0.391707	-1.506808	C	1.783675	1.372408	-0.724498
H	-2.499912	1.976176	-1.635563	H	1.562342	2.280824	-1.273347
H	-1.172528	2.908952	0.268630				
H	-0.640536	1.469697	2.246749				
H	-1.702759	-0.807230	2.487446				
H	-3.106651	-1.712141	0.591020				
H	4.711523	0.880691	0.481299				
H	3.548026	2.681329	-1.116794				



E: -481.952713

C	-3.378982	-0.936579	0.002136
C	-3.631678	0.431142	0.002623
C	-2.648715	1.458845	0.000240
C	-1.263833	1.319671	-0.002249
H	-4.187472	-1.658046	0.003362
Os	0.235698	-0.099489	-0.001246
H	-0.793198	2.309605	-0.005009

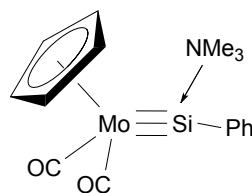
Effect of the Lewis Base on the Silicon Fragment

NMe₃

E: -174.471257

C	-0.802171	-1.133046	0.061452
N	0.000320	-0.000017	-0.374238
H	-0.880570	-1.216626	1.164964
H	-0.365225	-2.063835	-0.317751
C	1.382935	-0.127742	0.061603
H	1.973690	0.706141	-0.333982
H	1.496621	-0.133619	1.164957
H	1.808394	-1.060046	-0.326394
C	-0.580754	1.260867	0.061396
H	-1.590060	1.365399	-0.352561
H	-0.653938	1.351806	1.164417

H	0.025817	2.095664	-0.307331
H	-1.817027	-1.045233	-0.343363



NMe₂(CH₂)₂NMe₂

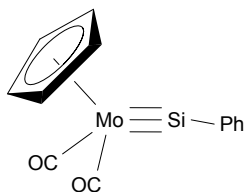
E: -347.739059

C	0.711675	-0.287863	0.973751
C	-0.711675	0.287835	0.973757
N	1.480847	-0.052240	-0.243372
N	-1.480841	0.052244	-0.243375
H	-0.668040	1.373792	1.124803
H	-1.219401	-0.125654	1.871865
H	1.219394	0.125596	1.871876
H	0.668036	-1.373824	1.124761
C	2.798741	-0.660584	-0.145625
H	3.327725	-0.551846	-1.098975
H	3.431658	-0.214226	0.648610
H	2.699511	-1.731244	0.067762
C	1.565833	1.353095	-0.614704
H	0.565858	1.738699	-0.827154
H	2.039360	1.985027	0.164529
H	2.163161	1.446443	-1.528333
C	-1.565847	-1.353090	-0.614721
H	-2.163180	-1.446418	-1.528349
H	-0.565876	-1.738701	-0.827177
H	-2.039383	-1.985024	0.164505
C	-2.798729	0.660602	-0.145614
H	-3.327695	0.551925	-1.098981
H	-3.431664	0.214206	0.648583
H	-2.699489	1.731249	0.067837

E: -897.792264

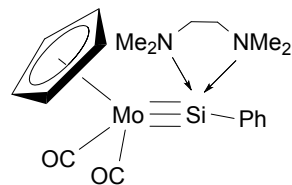
C	0.871179	-1.647163	1.322194
C	3.210429	1.285698	-0.666222
C	3.626125	0.010486	-1.138700
C	-3.083163	-0.588146	-1.216517
C	-2.982972	-0.703200	1.190674
C	3.609748	-0.053091	1.164342
C	3.201622	1.247210	0.758301
C	-2.377463	-0.325500	-0.024995
C	0.938630	-1.695730	-1.339354
C	-4.246364	-1.298105	1.216192
C	3.884769	-0.821115	-0.006416
C	-4.346065	-1.183287	-1.194491
C	-4.932364	-1.534616	0.023363
Mo	1.533120	-0.378237	-0.015479
O	0.543036	-2.411759	2.143775
O	0.653708	-2.491925	-2.145932
Si	-0.616438	0.370451	-0.051415
H	-2.452985	-0.551500	2.128401
H	-4.689648	-1.585310	2.166232
H	-5.913697	-2.001465	0.041582
H	-4.867356	-1.381123	-2.127659
H	-2.633895	-0.341522	-2.176169
H	2.955043	2.067035	1.420190
H	3.718723	-0.393619	2.185836
H	4.246869	-1.839877	-0.031298
H	3.753689	-0.271969	-2.175543

H	2.967386	2.140435	-1.283748	C	-5.580004	-0.019780	-0.244915
N	-1.263773	2.477108	0.002693	Mo	1.285411	0.007491	0.027893
C	-0.052593	3.321916	-0.110903	O	0.918888	2.335429	2.098496
H	0.649335	3.050375	0.679175	O	0.826464	-2.143812	2.261946
H	0.426137	3.139038	-1.074547	Si	-0.912389	0.015353	-0.333542
H	-0.321723	4.383407	-0.026961	H	-2.974774	2.158025	-0.392132
C	-2.187264	2.780612	-1.116161	H	-5.443872	2.131402	-0.347498
H	-3.082160	2.163104	-1.028500	H	-6.666514	-0.027673	-0.225531
H	-2.471386	3.841863	-1.103451	H	-5.409222	-2.168628	-0.145033
H	-1.689387	2.554638	-2.062958	H	-2.939848	-2.159836	-0.189349
C	-1.933055	2.739409	1.299671	H	2.201166	1.327081	-2.663638
H	-2.241749	3.791703	1.367958	H	3.530854	2.092494	-0.453414
H	-2.810875	2.096954	1.390908	H	4.240792	-0.128257	0.910477
H	-1.237970	2.514919	2.112980	H	3.317697	-2.269412	-0.460200
				H	2.066156	-1.368729	-2.666932



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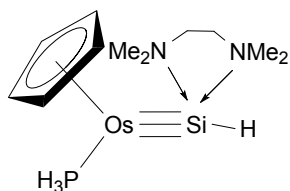
C	1.001995	1.454094	1.343301
C	2.533528	-0.757431	-1.906475
C	3.188657	-1.231938	-0.739144
C	-3.480029	-1.216943	-0.225818
C	-3.499543	1.207179	-0.339704
C	3.303861	1.073175	-0.737216
C	2.606027	0.669834	-1.905543
C	-2.769848	0.000381	-0.292851
C	0.944595	-1.324066	1.443910
C	-4.893194	1.195312	-0.314115
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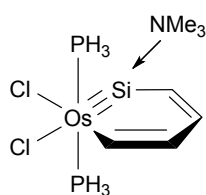
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C	2.999524	1.052860	-1.772034
C	-1.404364	2.510953	0.060156
C	-3.340453	1.114960	0.215265
C	3.609503	1.704074	0.351421
C	2.480900	2.485411	-0.038388
C	-1.935870	1.203820	0.118917
C	2.020036	-1.751371	-0.215434
C	-4.159188	2.245819	0.249411

H	0.560201	2.901551	-1.050758	H	3.740607	1.423907	-0.732827
H	-1.266829	3.124621	0.000009	H	3.979400	-0.870058	0.687785
Os	-0.708381	0.004406	-0.000180	H	2.165702	-0.837523	2.685388
C	3.216478	1.262452	0.000146	H	0.732629	1.454228	2.448726
C	3.924546	-0.713581	-1.215211	H	-1.715285	-0.877122	-1.832572
H	3.911824	-1.805013	-1.219267	H	2.019924	-3.044339	-1.133061
H	3.399325	-0.349696	-2.100400	H	0.607424	-2.247174	-2.499480
H	4.963630	-0.357490	-1.225027	H	2.631325	-1.601391	-2.549363
C	3.923064	-0.713481	1.216359	Os	1.190498	-0.065362	-0.079160
H	3.910281	-1.804916	1.220582	C	-1.918307	2.345995	0.349607
H	4.962162	-0.357464	1.227343	H	-1.863735	1.879594	1.332977
H	3.396813	-0.349453	2.100882	H	-0.914068	2.678149	0.083863
H	4.245766	1.643317	0.000921	H	-2.610140	3.198774	0.377438
H	2.692837	1.615005	-0.889355	C	-2.348920	2.009587	-1.998607
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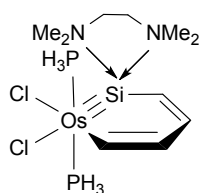
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Si	-0.890379	-0.194036	-0.781678	H	-1.874653	-0.677237	2.565140
C	3.253240	-0.087755	0.868688	H	-3.134424	-1.927242	2.816714
C	3.118649	1.121105	0.097749	C	-3.556513	-2.284245	0.141211
C	2.047575	1.876534	0.674272	H	-2.797133	-3.056736	-0.011351
C	1.524415	1.132025	1.786382	H	-4.396881	-2.721111	0.711368
C	2.277860	-0.088794	1.914334	H	-3.925067	-1.985595	-0.844665
N	-2.954249	-1.146310	0.827854	H	-4.033391	0.252593	-1.247078
N	-2.360619	1.355951	-0.663329	H	-4.429266	1.707830	-0.321019
H	1.722543	2.855568	0.349122	H	-4.893433	-0.261322	1.042622
				H	-3.552864	0.620466	1.760394



E: -470.887636

C	2.121028	2.282553	-0.040708
C	1.141073	3.283368	-0.074072
C	-0.271291	3.165200	-0.076657
C	-1.046535	2.003469	-0.046614
H	3.159641	2.599075	-0.038960
Os	-0.669820	0.036924	-0.008712
P	-0.939313	-0.332404	-2.332097
P	-1.094632	-0.195272	2.313389
H	0.095946	-0.921807	-3.116587
H	-2.004700	-1.214452	-2.644499
H	-1.259520	0.753656	-3.200338
H	-0.068322	-0.151165	3.309203
H	-2.006044	0.714737	2.915988
H	-1.695431	-1.430638	2.665183
Cl	-0.311979	-2.540306	-0.016763
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H	-2.121268	2.229029	-0.048755
H	-0.802640	4.117460	-0.102384
Si	1.460489	0.636151	-0.002397
H	1.508382	4.312308	-0.098887
C	2.946962	-1.518568	-1.134186
N	3.040703	-0.621493	0.063160
H	3.771326	-2.240840	-1.107019
H	3.025013	-0.914555	-2.042017
C	4.359588	0.066725	0.079090

H	4.421939	0.712571	0.956794
H	5.163261	-0.677701	0.113484
H	4.462887	0.673931	-0.822026
C	2.885631	-1.458635	1.296653
H	1.927373	-1.982256	1.240806
H	3.709236	-2.180534	1.347044
H	2.917346	-0.810533	2.176349
H	1.986374	-2.040909	-1.100883



E: -644.166718

C	-1.702288	-0.038955	2.307803
C	-0.715655	0.044807	3.272682
C	0.709273	0.144597	3.138438
C	1.458724	0.160722	1.977356
H	-2.730866	-0.094697	2.663921
Os	1.021030	0.003381	0.006200
P	1.435826	-2.309406	0.153583
P	1.498329	2.295759	-0.324565
H	1.516606	-3.068089	-1.051950
H	2.695513	-2.642332	0.719601
H	0.634917	-3.225782	0.910210
H	0.640861	3.390487	0.036534
H	2.669101	2.768546	0.326968
H	1.785041	2.712272	-1.655892
Cl	0.536176	-0.226852	-2.558971
Cl	3.524641	-0.023157	-0.440136
H	2.535482	0.259860	2.176196

H	1.241713	0.220620	4.088246
Si	-1.143308	-0.002570	0.581473
H	-1.061166	0.043072	4.310894
C	-3.757517	0.719122	-0.631374
C	-3.386236	-0.599948	-1.288007
N	-2.515423	1.448362	-0.266629
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H	-2.798620	-0.425491	-2.192735
H	-4.284488	-1.166018	-1.568732
H	-4.377238	1.327153	-1.303909
H	-4.332171	0.551351	0.284016
C	-2.816305	2.510968	0.727909
H	-1.883572	2.992906	1.025611
H	-3.491245	3.258035	0.290455
H	-3.269104	2.068277	1.615374
C	-1.913719	2.074349	-1.484919
H	-1.406144	1.329451	-2.103803
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H	-1.165583	2.797841	-1.166470
C	-3.380840	-2.090184	0.655624
H	-2.732037	-2.551612	1.401055
H	-4.032421	-1.382129	1.168368
H	-3.994918	-2.857233	0.166385
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H	-1.280071	-3.089436	-0.452860
H	-2.514231	-3.019105	-1.729420
H	-1.078317	-1.926304	-1.797882