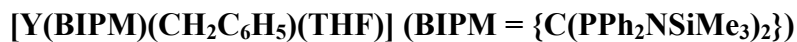


- *Supplementary Information* -

## Synthesis and Reactivity of the Yttrium-Alkyl-Carbene Complex



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### Coordinates and Energy for 3

1.H	-0.723398	3.189830	-5.196961
2.H	0.104368	1.633085	-4.946057
3.H	2.216987	-1.670344	-4.842984
4.H	4.669359	-1.500727	-4.430888
5.C	-0.171175	2.581712	-4.461246
6.H	-3.363070	2.191150	-4.243971
7.H	0.758815	3.120181	-4.225381
8.H	-2.828988	-2.149097	-3.982091
9.C	2.593530	-1.043598	-4.031999
10.H	-2.694197	0.561637	-4.006488
11.C	3.969469	-0.945948	-3.803479
12.H	-2.484359	-3.865326	-3.637495
13.C	-2.873521	1.528848	-3.511254
14.H	0.624876	-0.391643	-3.403068
15.H	-4.997743	-2.941823	-3.116086
16.C	-2.786329	-2.909933	-3.188878
17.C	1.699423	-0.336377	-3.223452
18.H	-2.206003	4.638185	-3.023323
19.Si	-1.251345	2.328304	-2.919310
20.C	4.445334	-0.139307	-2.763658
21.H	-3.587870	1.367122	-2.688588
22.H	5.518372	-0.063882	-2.579594
23.C	-4.130526	-2.987029	-2.444436
24.H	2.668903	3.061684	-2.765578

25.H	3.321866	5.442520	-2.547661
26.H	-0.962629	-1.904777	-2.429051
27.C	-1.696636	4.045172	-2.245994
28.H	-4.193535	-3.918056	-1.862275
29.C	2.165516	0.467319	-2.171852
30.H	-0.799465	4.601309	-1.931805
31.C	-1.838412	-2.466893	-2.081894
32.C	3.550615	0.556705	-1.947998
33.H	-4.446025	-0.863567	-2.001592
34.C	2.348385	3.630741	-1.891543
35.C	2.716923	4.974869	-1.769099
36.N	-0.543995	1.272151	-1.710329
37.H	-1.505603	-3.313462	-1.461861
38.C	-4.068587	-1.775358	-1.518884
39.H	-2.369274	3.982439	-1.376348
40.H	4.752185	-4.484223	-1.041564
41.H	-6.469339	1.650305	-1.237109
42.H	2.303175	-4.935883	-1.148062
43.O	-2.634168	-1.568659	-1.238595
44.H	3.928911	1.174453	-1.131408
45.P	0.964653	1.273768	-1.028840
46.C	4.048982	-3.807678	-0.552530
47.C	1.583815	3.008066	-0.892151
48.C	2.674837	-4.058968	-0.614270
49.H	-4.581794	-1.912501	-0.559572
50.H	2.595601	6.765048	-0.562481
51.C	2.312563	5.714956	-0.654327
52.H	-4.308206	2.569469	-0.494496
53.C	-5.973294	1.211067	-0.369135
54.H	-7.551752	-0.231594	0.009679
55.H	5.590629	-2.477010	0.176448
56.C	4.519213	-2.679929	0.129968
57.C	-4.743951	1.724008	0.043355
58.C	1.776295	-3.188317	0.009096
59.H	0.703167	-3.380173	-0.021955
60.C	-6.583589	0.157790	0.325401
61.Y	-1.508160	0.107411	0.150288
62.C	1.196963	3.755810	0.232617
63.C	1.549171	5.101775	0.347066
64.C	0.814097	0.567543	0.490729
65.C	3.620236	-1.803455	0.741765
66.C	2.237314	-2.052483	0.691959
67.H	0.621365	3.259740	1.015944
68.H	1.232573	5.674086	1.220812
69.H	3.993516	-0.919783	1.263262
70.H	-2.572523	-3.960048	1.115582
71.C	-4.062100	1.220116	1.190395
72.C	-5.928286	-0.372448	1.445330
73.H	-2.528155	2.735653	1.270753
74.P	1.026418	-0.845121	1.381105

75.C	-2.749135	1.708137	1.583565
76.N	-0.462105	-1.555200	1.509640
77.H	-6.389085	-1.184896	2.010973
78.H	-3.479521	-2.585598	1.799074
79.C	-4.698423	0.135154	1.862879
80.C	-2.738501	-3.367313	2.028663
81.H	0.288309	-4.699798	2.225772
82.H	-2.493303	1.542907	2.636800
83.H	-3.189678	-4.034918	2.781034
84.H	-4.226242	-0.273492	2.759347
85.Si	-1.116062	-2.648581	2.714649
86.C	0.014879	-4.119478	3.119875
87.C	1.680654	-0.470785	3.067002
88.H	0.674873	1.431329	3.092184
89.H	2.809082	-2.298616	3.339750
90.H	0.946734	-3.795797	3.607115
91.H	-0.501654	-4.797660	3.819319
92.C	1.279638	0.732055	3.672217
93.C	2.479547	-1.364754	3.797242
94.H	-2.242013	-0.946171	4.196208
95.C	-1.544087	-1.784270	4.348511
96.H	-0.645114	-1.381264	4.840826
97.H	-2.019440	-2.495649	5.043597
98.C	1.653715	1.027511	4.984347
99.C	2.869461	-1.061658	5.106475
100.H	1.325817	1.960733	5.445847
101.H	3.499726	-1.760831	5.658405
102.C	2.452354	0.130828	5.705292
103.H	2.751970	0.363537	6.728679

Energy: -614.03733565 eV