

- *Supplementary Information* -

**Synthesis and Structure of a bis-N-Heterocyclic Carbene Complex of Uranium  
Tetrachloride Exhibiting Short Cl...C<sub>carbene</sub> Contacts**

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**Coordinates and energy for 1a:**

1.H	-1.435651	0.031194	-5.917734
2.H	-3.945575	0.423457	-5.446200
3.H	-1.318589	2.101261	-5.344617
4.H	-1.394919	-1.526393	-5.073221
5.H	3.312868	-0.830301	-5.001620
6.H	-3.914209	-1.258693	-4.859552
7.C	-1.320348	-0.439663	-4.929539
8.H	-1.079809	4.469771	-4.677845
9.C	-3.803083	-0.207039	-4.554769
10.H	3.068680	0.853547	-4.495977
11.H	-0.315435	-0.219451	-4.549025
12.C	-1.669206	2.420179	-4.363544
13.C	2.994627	-0.191696	-4.163683
14.H	3.722725	-2.806972	-4.181358
15.H	5.701107	-0.926767	-4.005285
16.C	-1.533437	3.755280	-3.989299
17.H	1.942231	-0.403845	-3.939665
18.H	-4.606647	0.023530	-3.842254
19.C	-2.404154	0.024151	-3.944980
20.H	5.500350	0.817114	-3.705599
21.C	-2.231529	1.473810	-3.496325
22.C	5.358147	-0.183223	-3.269203
23.H	3.375976	-5.058682	-3.214435

24.C	3.610794	-2.918765	-3.102208
25.H	-5.010739	-3.625140	-2.775571
26.H	-2.310178	-0.610659	-3.053203
27.C	3.872647	-0.406309	-2.918743
28.C	-1.969171	4.176988	-2.736932
29.H	-2.612541	-4.469696	-2.734919
30.C	3.414241	-4.185787	-2.560964
31.H	-1.857209	5.224200	-2.454226
32.H	6.007178	-0.261745	-2.385881
33.C	3.650244	-1.777257	-2.287390
34.H	3.573744	0.353420	-2.184380
35.C	-2.645769	1.928929	-2.223413
36.C	-5.003978	-3.496411	-1.682658
37.C	-2.541403	3.277802	-1.823983
38.H	-5.322873	1.523259	-1.762237
39.C	-2.673707	-4.463605	-1.637299
40.H	-5.649144	-2.641011	-1.440045
41.Cl	-0.018888	-1.995240	-1.786131
42.Cl	0.883746	1.559200	-1.760270
43.H	-5.449185	-4.396156	-1.230519
44.H	-3.087977	-5.435085	-1.328427
45.H	-4.333783	5.365079	-1.311806
46.H	-3.157993	-2.385108	-1.644057
47.H	2.391630	4.748615	-1.426527
48.C	3.255814	-4.339423	-1.185374
49.C	-3.559550	-3.294468	-1.177215
50.C	-4.654093	0.875088	-1.211393
51.N	-3.270586	0.976838	-1.317075
52.H	-1.654021	-4.369423	-1.244837
53.H	-5.177712	3.816478	-1.110917
54.H	3.091103	-5.334832	-0.773392
55.H	4.822064	4.537544	-0.735116
56.C	3.488326	-1.965252	-0.898962
57.C	-4.429187	4.482780	-0.660234
58.C	-3.061157	3.789889	-0.483665
59.H	-1.954711	5.683508	-0.343763
60.C	2.113391	4.588551	-0.375067
61.C	-2.631516	0.043583	-0.533129
62.C	-4.905483	-0.141377	-0.347183
63.C	3.297204	-3.238626	-0.318329
64.H	3.150011	2.725134	-0.327556
65.H	1.101442	4.167575	-0.358989
66.H	-5.837739	-0.556905	0.012466
67.H	2.098039	5.572477	0.117719
68.H	5.791401	-0.847509	0.041614
69.H	-4.815718	4.819684	0.313380
70.C	4.526532	4.267144	0.290034
71.N	3.622933	-0.811044	-0.020419
72.H	-3.193947	2.923952	0.178493
73.N	-3.670093	-0.641937	0.052584

74.U	-0.009192	-0.125587	-0.007729
75.C	-2.078875	4.744115	0.215379
76.C	3.120282	3.633475	0.288534
77.C	-3.536081	-3.084589	0.334574
78.C	4.880623	-0.368598	0.377161
79.H	5.288115	3.585116	0.692969
80.H	-1.096922	4.275072	0.345871
81.H	4.539859	5.183832	0.899762
82.H	-3.466061	-5.193918	0.774917
83.C	2.617543	-0.051824	0.532671
84.C	-3.579777	-1.802914	0.926649
85.H	-2.462071	5.003176	1.212981
86.C	-3.516677	-4.190199	1.196968
87.H	1.245153	-4.471463	1.062710
88.H	2.632538	-5.573308	1.307025
89.C	4.678300	0.688797	1.204108
90.C	3.175502	-3.446747	1.188600
91.H	5.024568	-4.595489	1.414889
92.N	3.301980	0.869777	1.291848
93.H	5.375930	1.319486	1.739469
94.C	2.214979	-4.587357	1.561593
95.H	5.242950	-2.846220	1.661832
96.H	2.755131	-2.526671	1.615868
97.C	2.694151	3.226829	1.696219
98.C	4.558036	-3.688594	1.829858
99.Cl	-0.738986	1.731445	1.633962
100.Cl	-0.048677	-1.853361	1.921381
101.H	2.174591	5.242994	2.260246
102.C	2.747031	1.897004	2.162545
103.H	-5.789614	0.180068	2.420817
104.C	-3.624518	-1.607814	2.322654
105.H	-3.306673	0.499376	2.225365
106.C	-3.557980	-4.029153	2.580184
107.H	2.036329	-4.577318	2.645904
108.C	2.238890	4.206202	2.592430
109.H	4.452904	-3.825954	2.916707
110.H	-3.537852	-4.904500	3.230973
111.C	-3.690162	-0.222727	2.958849
112.C	-3.614656	-2.752746	3.132920
113.C	-5.140721	0.169018	3.307453
114.H	2.313016	-0.568352	3.116667
115.H	-5.164680	1.173854	3.755856
116.C	2.368625	1.531742	3.473602
117.H	4.648302	-0.060190	3.877713
118.H	-5.571444	-0.538116	4.033224
119.C	1.856716	3.877227	3.889340
120.H	-3.633677	-2.638117	4.216804
121.C	2.452258	0.094671	3.981339
122.H	-1.780350	-0.463134	3.988581
123.C	-2.795582	-0.107706	4.204226

124.C	1.919291	2.553906	4.320618
125.H	1.498329	4.654009	4.566245
126.C	3.833579	-0.204333	4.600209
127.H	-2.732511	0.942854	4.520186
128.H	0.354908	0.033948	4.597814
129.H	3.873717	-1.247097	4.949748
130.H	-3.197491	-0.684554	5.051115
131.C	1.340846	-0.251841	4.983988
132.H	1.331716	-1.335635	5.164361
133.H	4.021881	0.452704	5.463480
134.H	1.602377	2.305509	5.333162
135.H	1.495775	0.242650	5.955014

**Energy:** -794.82352869 eV