Supplementary Material for Chemical Communications

A Computational Study of the Reactions of a β-Diketiminatoaluminium (I) Complex with the Hydrogen Atom and the Electron

Iain McKenzie, Paul W. Percival, and Jason A. C. Clyburne*

[a] *Department of Chemistry, Simon Fraser University, 8888 University Drive, Burnaby BC V5A 1S6, Canada. E-mail: clyburne@sfu.ca*

Supporting Information

Aluminum carbene analogue (**2**)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000000	-1.925846	-0.000003
2	7	0	-1.413868	-0.527439	0.000000
3	7	0	1.413868	-0.527439	0.000001
4	6	0	-1.260017	0.801968	0.000000
5	6	0	0.000000	1.425720	-0.000001
6	6	0	1.260017	0.801968	0.000000
7	6	0	-2.476072	1.705766	0.000001
8	6	0	2.476072	1.705766	-0.000001
9	6	0	-2.776219	-1.075501	0.000002
10	6	0	2.776218	-1.075502	0.000003
11	1	0	0.000000	2.508584	-0.000002
12	1	0	-2.183464	2.756903	-0.000003
13	1	0	-3.102285	1.523994	0.880607
14	1	0	-3.102291	1.523989	-0.880601
15	1	0	2.183464	2.756903	0.000001
16	1	0	3.102287	1.523992	-0.880606
17	1	0	3.102290	1.523991	0.880601
18	1	0	-3.344785	-0.776051	-0.889284
19	1	0	-3.344785	-0.776046	0.889285
20	1	0	-2.707747	-2.167556	0.000005
21	1	0	3.344783	-0.776051	0.889289
22	1	0	3.344787	-0.776049	-0.889280
23	1	0	2.707745	-2.167557	0.000002

N-N= 5.941728538055D+02 E-N=-2.656260499170D+03 KE= 6.217978046777D+02
1\1\GINC-B060\FOpt\UB3LYP\6-31++G(d,p)\C7H13Al1N2\IMCKENZI\23-Mar-2003
\0\\# UB3LYP/6-31++G(D,P) OPT(TIGHT) FORMCHECK=(ALL) POP=(MINIMAL)\\Al
uminum carbene analogue.\\0,1\Al,0.0006921695,-1.9236697353,-0.0915346
158\N,-1.4136127036,-0.5279985639,-0.0114806955\N,1.4139917054,-0.5256
880016,-0.0386549487\C,-1.2602465024,0.8000318154,0.0502246812\C,-0.00
05124122,1.4241091219,0.0677606486\C,1.2596701779,0.8020910275,0.02600
70727\C,-2.476569645,1.7018147072,0.1048678962\C,2.4753438546,1.705861
1189,0.0572757019\C,-2.7757031402,-1.0765540893,-0.0244352043\C,2.7764
759166,-1.0720178631,-0.077793526\H,-0.0009017839,2.5057487988,0.11922
65136\H,-2.1843529259,2.7520035377,0.1520107763\H,-3.0942015919,1.4778
883616,0.981816866\H,-3.1111816223,1.5615801716,-0.7773189277\H,2.1823
717984,2.7555716191,0.1100476677\H,3.0931072819,1.5666532273,-0.836950
9957\H,3.1100856227,1.4829549387,0.9221845084\H,-3.3529214196,-0.73564
62957,-0.8929784478\H,-3.3357797804,-0.8201632549,0.8834986805\H,-2.70
68415176,-2.1673191302,-0.0769935312\H,3.3534773186,-0.8147018378,0.81
92148912\H,3.3363392944,-0.7301780657,-0.9572620325\H,2.708398596,-2.1
628945835,-0.1290400763\\Version=x86-Linux-G98RevA.11.3\HF=-626.573965
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2-H1

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.000001	-1.618132	-0.000039
2	7	0	1.465644	-0.577027	-0.007624
3	7	0	-1.465647	-0.577029	0.007607
4	1	0	0.000004	-3.190094	-0.000092
5	6	0	1.279345	0.831997	0.018169
6	6	0	-1.279346	0.831996	-0.018156
7	6	0	2.822001	-1.109010	-0.117759
8	6	0	-2.821998	-1.109008	0.117843
9	6	0	0.000000	1.405890	0.000010
10	6	0	2.495638	1.713600	0.130330
11	6	0	-2.495637	1.713599	-0.130355
12	1	0	3.467145	-0.786719	0.709414
13	1	0	3.309310	-0.817666	-1.059083
14	1	0	2.785595	-2.203261	-0.094525
15	1	0	-3.467214	-0.786687	-0.709261
16	1	0	-3.309220	-0.817691	1.059221
17	1	0	-2.785600	-2.203259	0.094568
18	1	0	-0.000002	2.492097	0.000011
19	1	0	2.198759	2.764413	0.091814
20	1	0	3.221112	1.548294	-0.677449
21	1	0	3.038716	1.563800	1.076345
22	1	0	-2.198763	2.764412	-0.091794
23	1	0	-3.221156	1.548270	0.677378
24	1	0	-3.038659	1.563821	-1.076405

Total atomic spin densities:

1	Al	-0.015643
2	N	0.104898
3	N	0.104896
4	H	-0.000449
5	C	0.455941
6	C	0.455931
7	C	-0.004244
8	C	-0.004246
9	C	-0.182120
10	C	-0.029344
11	C	-0.029314
12	H	0.004056
13	H	0.014675
14	H	-0.000733
15	H	0.004053
16	H	0.014681
17	H	-0.000733
18	H	0.007619
19	H	0.000434
20	H	0.017952
21	H	0.031650

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 22  H    0.000434
 23  H    0.017948
 24  H    0.031655

N-N= 6.118823330696D+02 E-N=-2.696111015702D+03  KE= 6.243446957909D+02
 1\1\GINC-B010\SP\UB3LYP\Gen\C7H14Al1N2(2)\IMCKENZI\03-Jun-2003\0\\# UB
 3LYP SCF=TIGHT GEN FORMCHECK=(ALL) POP=(MINIMAL)\\Single point of the
 H adduct of the aluminum in the aluminum carbene analogue.\\0,2\Al\N,1
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 42152134,1,117.84537467,2,1.13218039,0\C,2,1.46110943,1,123.11132507,5
 ,-176.29872269,0\C,3,1.46110888,1,123.11146185,6,-176.29484537,0\C,5,1
 .40228645,2,121.66745969,1,-2.33621297,0\C,5,1.50637802,2,118.40066802
 ,9,177.22110506,0\C,6,1.50637844,3,118.40053673,1,174.88101919,0\H,7,1
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 4,12,-121.91341253,0\H,7,1.09510299,2,109.35085902,12,119.0636246,0\H,
 8,1.09740451,3,112.45705835,1,-124.41795879,0\H,8,1.09929291,3,112.306
 4035,15,-121.91334727,0\H,8,1.09510307,3,109.35087871,15,119.06366349,
 0\H,9,1.08620762,5,114.15808621,2,-178.65333173,0\H,10,1.09262424,5,10
 9.92794678,2,177.42012969,0\H,10,1.09824688,5,112.98640425,19,-119.899
 19713,0\H,10,1.10105246,5,112.49488563,19,119.33650865,0\H,11,1.092624
 37,6,109.92799134,3,177.41930834,0\H,11,1.09824606,6,112.98663912,22,-
 119.89940368,0\H,11,1.10105363,6,112.49454535,22,119.33635545,0\\Versi
 on=x86-Linux-G98RevA.11.3\HF=-627.2861544\S2=0.76925\S2-1=0.\S2A=0.750
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 14Al1N2)]\\@
```

2-H2

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.269889	-1.820412	-0.792241
2	7	0	1.355990	-0.371627	-0.117329
3	7	0	-1.459759	-0.805061	0.067808
4	6	0	0.996863	0.944440	0.045458
5	6	0	-0.339801	1.373359	-0.120528
6	6	0	-1.490850	0.614175	-0.253188
7	6	0	2.053082	1.991180	0.314027
8	6	0	-2.841188	1.192285	-0.565131
9	6	0	2.769213	-0.722716	0.051846
10	6	0	-1.526872	-1.085097	1.532499
11	1	0	-2.261730	-1.259059	-0.369341
12	1	0	-0.482995	2.449389	-0.174193
13	1	0	1.597266	2.979497	0.409430
14	1	0	2.797430	2.041542	-0.492227
15	1	0	2.606527	1.792231	1.240673
16	1	0	-2.770150	2.268359	-0.746305
17	1	0	-3.564384	1.037670	0.250874
18	1	0	-3.281298	0.740667	-1.467348
19	1	0	3.434220	-0.155379	-0.612154
20	1	0	2.899265	-1.785093	-0.185769
21	1	0	3.114357	-0.576697	1.084606
22	1	0	-2.428789	-0.656269	1.983148
23	1	0	-0.646146	-0.651059	2.007250
24	1	0	-1.518435	-2.169386	1.687239

N-N= 6.111620623265D+02 E-N=-2.691422326123D+03 KE= 6.223130787271D+02
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003\0\\# UB3LYP/6-31++G(D,P) OPT FORMCHECK=(ALL) POP=(MINIMAL)\\Additi
on of H to N2 of the aluminum carbene analogue.\\0,2\Al,-0.0811879825,
-0.7538922532,1.8545819373\N,1.2671747225,-0.2765227576,0.5553514664\N
,-1.5320213731,0.2833174946,0.5969042461\C,1.1107394679,-0.1167852837,
-0.8002342759\C,-0.167171927,-0.1256213899,-1.4043996557\C,-1.41625816
11,-0.0822349787,-0.8071191576\C,2.3228033354,-0.0237904827,-1.6978320
936\C,-2.7070295416,-0.2393299769,-1.5582305317\C,2.6310591205,-0.2771
542457,1.09281275\C,-1.442113338,1.7537126519,0.8379728517\H,-2.437770
1999,-0.0308204767,0.9452284628\H,-0.1719346092,-0.199441538,-2.488747
6166\H,2.0189524784,0.0934047173,-2.7406891083\H,2.9544258289,-0.92004
63361,-1.6312095199\H,2.9621917444,0.8309301337,-1.4423848943\H,-2.518
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89143148\H,-3.3183100315,-1.0608297123,-1.1542544924\H,3.272194352,-1.
0409659187,0.6339473038\H,2.5863280899,-0.490874537,2.167205911\H,3.12
56277173,0.6969302859,0.9761453381\H,-2.2117135953,2.3003484004,0.2817
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=0.763335\S2-1=0.\S2A=0.750065\RMSD=6.894e-09\RMSF=1.121e-05\Dipole=-0
.4318964,0.8540321,-0.8668733\PG=C01 [X(C7H14Al1N2)]\\@

Supplementary Material for Chemical Communications

2-H3

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.233667	-1.627847	-0.024067
2	7	0	1.312823	-0.677649	0.168413
3	7	0	-1.561766	-0.452373	-0.295729
4	6	0	1.291989	0.667833	-0.263056
5	6	0	0.149167	1.380392	-0.418030
6	6	0	-1.284273	0.986377	-0.103870
7	6	0	2.621173	1.298433	-0.624291
8	6	0	-1.693839	1.481213	1.304076
9	6	0	2.569323	-1.253534	0.642473
10	6	0	-2.953026	-0.763134	-0.586471
11	1	0	0.258287	2.391625	-0.800023
12	1	0	-1.917559	1.523870	-0.830357
13	1	0	2.472945	2.325291	-0.964426
14	1	0	3.122243	0.742600	-1.426730
15	1	0	3.308796	1.324717	0.228793
16	1	0	-1.581187	2.569015	1.377891
17	1	0	-1.055228	1.021375	2.065729
18	1	0	-2.737899	1.234079	1.528214
19	1	0	2.949329	-0.736371	1.535089
20	1	0	3.362657	-1.245685	-0.116447
21	1	0	2.400126	-2.298871	0.921113
22	1	0	-3.291216	-0.255427	-1.504025
23	1	0	-3.636387	-0.468697	0.224575
24	1	0	-3.077706	-1.840838	-0.740297

N-N= 6.163211399424D+02 E-N=-2.702528221860D+03 KE= 6.223563545775D+02
1\1\GINC-B034\FOpt\UB3LYP\6-31++G(d,p)\C7H14Al1N2(2)\IMCKENZI\21-Mar-2
003\0\\# UB3LYP/6-31++G(D,P) OPT(TIGHT) FORMCHECK=(ALL) POP=(MINIMAL)\
\Addition of H to C3 of the aluminum carbene analogue.\\0,2\Al,-0.2337
137753,-1.6278400803,-0.0240674592\N,1.3128034732,-0.6776862339,0.1684
127017\N,-1.5617792552,-0.4523284291,-0.2957290802\C,1.2920078387,0.66
77960024,-0.2630560625\C,0.1492060051,1.3803876333,-0.4180295731\C,-1.
2842449895,0.9864140973,-0.1038697501\C,2.621209872,1.2983578689,-0.62
42906244\C,-1.6937968534,1.4812613323,1.3040755485\C,2.5692872611,-1.2
536075084,0.642473062\C,-2.9530477479,-0.763049854,-0.5864707576\H,0.2
583558839,2.391617374,-0.800022681\H,-1.9175152421,1.5239250448,-0.830
3568098\H,2.4730114995,2.3252197486,-0.9644259195\H,3.1222645453,0.742
5110919,-1.4267304523\H,3.3088336163,1.3246224554,0.2287929032\H,-1.58
11136636,2.5690605595,1.3778911135\H,-1.05519873,1.0214047385,2.065729
179\H,-2.7378632239,1.2341572423,1.5282142021\H,2.9493079863,-0.736455
2798,1.535089287\H,3.3626214167,-1.2457816958,-0.116446716\H,2.4000599
098,-2.2989395829,0.9211134115\H,-3.2912234034,-0.2553331423,-1.504025
307\H,-3.6364005259,-0.4685927149,0.2245751855\H,-3.0777588334,-1.8407
495854,-0.7402968332\\Version=x86-Linux-G98RevA.11.3\HF=-627.1346485\S
2=0.752361\S2-1=0.\S2A=0.750003\RMSD=3.730e-09\RMSF=8.055e-07\Dipole=0
.2077388,-0.2494192,0.0420074\PG=C01 [X(C7H14Al1N2)]\\@

H-C4

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000005	-1.956178	-0.540029
2	7	0	-1.397311	-0.553252	-0.064200
3	7	0	1.397317	-0.553246	-0.064207
4	6	0	-1.217265	0.746818	-0.237413
5	6	0	-0.000003	1.128682	-1.036697
6	6	0	1.217264	0.746824	-0.237419
7	6	0	-2.129531	1.796083	0.339185
8	6	0	2.129516	1.796093	0.339196
9	6	0	-2.571479	-1.025522	0.671555
10	6	0	2.571487	-1.025511	0.671549
11	1	0	-0.000004	0.553515	-1.988597
12	1	0	-0.000006	2.195262	-1.271654
13	1	0	-1.751332	2.800549	0.135547
14	1	0	-3.136925	1.724284	-0.095769
15	1	0	-2.252467	1.694409	1.425778
16	1	0	1.751385	2.800560	0.135435
17	1	0	2.252322	1.694503	1.425813
18	1	0	3.136955	1.724210	-0.095633
19	1	0	-3.506057	-0.674688	0.215377
20	1	0	-2.560417	-0.701724	1.720394
21	1	0	-2.574952	-2.119753	0.658524
22	1	0	2.560444	-0.701678	1.720377
23	1	0	3.506065	-0.674706	0.215346
24	1	0	2.574944	-2.119743	0.658552

N-N= 6.127211275696D+02 E-N=-2.694352536209D+03 KE= 6.223172946883D+02
1\1\GINC-B002\FOpt\UB3LYP\6-31++G(d,p)\C7H14Al1N2(2)\IMCKENZI\15-Apr-2
003\0\\# UB3LYP/6-31++G(D,P) OPT FORMCHECK=(ALL) POP=(MINIMAL)\\H addi
tion to C4 ob the aluminum carbene analogue. (chair conformation)\\0,2
\Al,0.061226729,-1.5512796991,1.306921796\N,1.4129765649,-0.446604358,
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,0.8028982589,-0.1228522941\C,-0.0199869136,1.458275021,0.4708472825\C
,-1.2350328337,0.7521778176,-0.0690517935\C,2.0741102194,1.5341302725,
-1.1047061746\C,-2.1829721406,1.4453896128,-1.0106048725\C,2.591531778
,-1.1584616517,-0.2389869727\C,-2.5490611457,-1.2656115479,-0.12533756
91\H,0.007041257,1.3334643928,1.5756653284\H,-0.0473467611,2.525234327
1,0.2392270492\H,1.6701158301,2.5237056115,-1.3305019023\H,3.088009643
2,1.6715953299,-0.7018487634\H,2.1874906813,0.9904401971,-2.0521662466
\H,-1.8309847939,2.4507766627,-1.2530023885\H,-2.315223182,0.896645738
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\H,2.6259661836,-2.1468733899,0.2293928855\H,-2.5590760302,-1.40935486
6,-1.2135787089\H,-3.4878969112,-0.7758691416,0.1633862982\H,-2.521554
2145,-2.2541825188,0.3431642631\\Version=x86-Linux-G98RevA.11.3\HF=-62
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6\Dipole=-0.0633683,1.4588838,-1.4912423\PG=C01 [X(C7H14Al1N2)]\\@

Radical anion (**2**$^{-}$)

Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000000	0.000000	-1.863143
2	7	0	0.000000	1.426770	-0.572585
3	7	0	0.000000	-1.426770	-0.572585
4	6	0	-0.008818	1.268781	0.814048
5	6	0	0.008818	-1.268781	0.814048
6	6	0	-0.161797	2.775368	-1.091617
7	6	0	0.161797	-2.775368	-1.091617
8	6	0	0.000000	0.000000	1.413566
9	6	0	0.180520	2.478009	1.702325
10	6	0	-0.180520	-2.478009	1.702325
11	1	0	0.617961	3.474683	-0.750452
12	1	0	-1.139949	3.226196	-0.829618
13	1	0	-0.110051	2.735969	-2.186859
14	1	0	-0.617961	-3.474683	-0.750452
15	1	0	1.139949	-3.226196	-0.829618
16	1	0	0.110051	-2.735969	-2.186859
17	1	0	0.000000	0.000000	2.501659
18	1	0	0.058753	2.197197	2.753660
19	1	0	-0.528571	3.287642	1.491394
20	1	0	1.193153	2.920933	1.600343
21	1	0	-0.058753	-2.197197	2.753660
22	1	0	0.528571	-3.287642	1.491394
23	1	0	-1.193153	-2.920933	1.600343

Total atomic spin densities:

1	Al	-0.008576
2	N	0.134494
3	N	0.134494
4	C	0.235083
5	C	0.235083
6	C	0.008086
7	C	0.008086
8	C	-0.168356
9	C	0.193534
10	C	0.193534
11	H	-0.016796
12	H	0.037133
13	H	-0.000752
14	H	-0.016796
15	H	0.037133
16	H	-0.000752
17	H	0.006001
18	H	-0.021323
19	H	-0.030836
20	H	0.046845
21	H	-0.021323

```
 22  H   -0.030836
 23  H    0.046845

1\1\GINC-B091\SP\UB3LYP\Gen\C7H13Al1N2(1-,2)\IMCKENZI\02-Jun-2003\0\\#
  UB3LYP SCF=TIGHT GEN FORMCHECK=(ALL) POP=(MINIMAL)\\Radical anion of
 the aluminum carbene analogue.\\-1,2\Al\N,1,1.92385377\N,1,1.92385377,
 2,95.73935489\C,2,1.39563289,1,125.62941768,3,-0.44536742,0\C,3,1.3956
 3288,1,125.62942099,2,-0.44536745,0\C,2,1.45405949,1,116.63981419,4,-1
 72.40346706,0\C,3,1.45405942,1,116.63981596,5,-172.40346004,0\C,4,1.40
 331908,2,121.78740526,1,0.90734447,0\C,4,1.51232145,2,119.48964357,8,1
 70.87544413,0\C,5,1.51232136,3,119.48964108,1,171.78278206,0\H,6,1.101
 57082,2,113.54529087,1,-127.5541235,0\H,6,1.10845407,2,113.01917718,11
 ,-122.18744188,0\H,6,1.0971711,2,108.52830674,11,119.31008,0\H,7,1.101
 57082,3,113.545292,1,-127.55417966,0\H,7,1.10845402,3,113.01918111,14,
 -122.18743196,0\H,7,1.09717111,3,108.52831313,14,119.31008728,0\H,8,1.
 08809356,4,115.29087208,2,179.52111068,0\H,9,1.09498342,4,110.17982979
 ,2,174.96928859,0\H,9,1.09672527,4,113.35102093,18,-120.61199352,0\H,9
 ,1.10995801,4,112.29175961,18,119.13737221,0\H,10,1.09498342,5,110.179
 83306,3,174.96929094,0\H,10,1.09672521,5,113.35102291,21,-120.61199414
 ,0\H,10,1.10995805,5,112.29176368,21,119.13737057,0\\Version=x86-Linux
 -G98RevA.11.3\State=2-A\HF=-626.702426\S2=0.765623\S2-1=0.\S2A=0.75009
 4\RMSD=1.967e-09\Dipole=1.4231548,0.,1.2872878\PG=C02 [C2(Al1C1H1),X(C
 6H12N2)]\\@
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