Supporting information for:

The Final Fate of NHC stabilized Dicarbon

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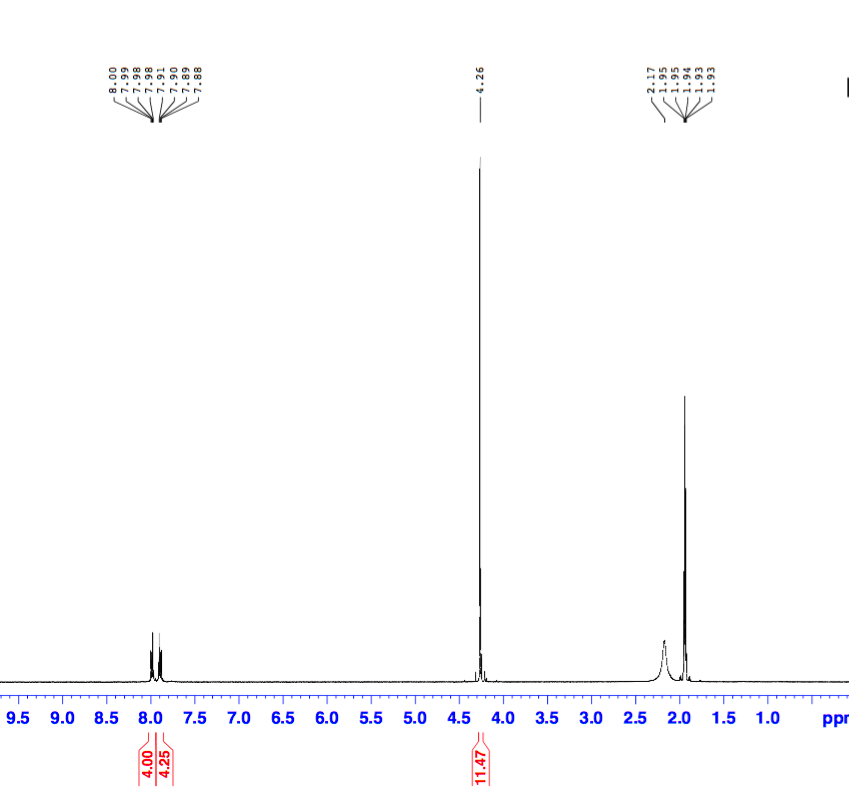
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Figure S1. 1H NMR spectrum of **14**.

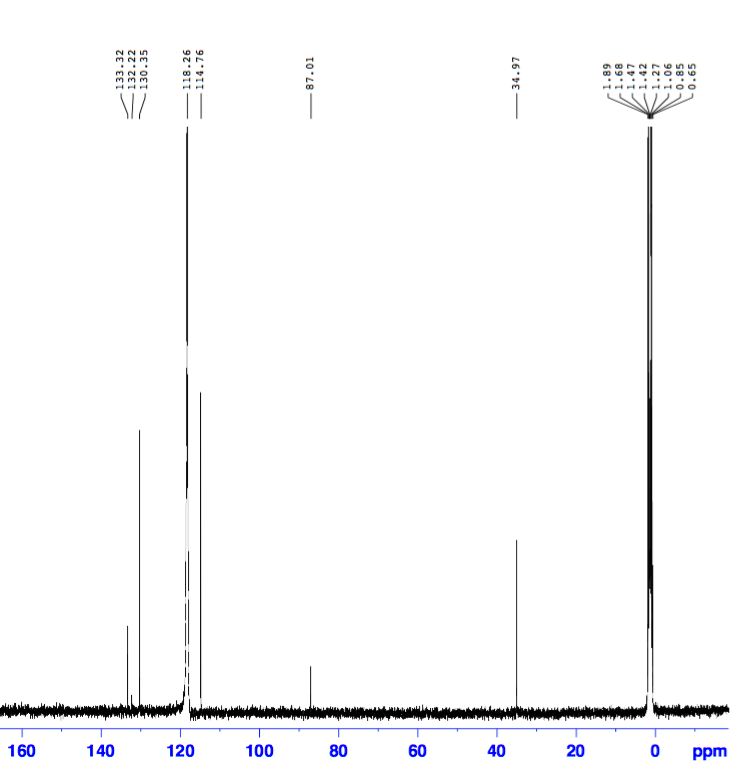
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Figure S2. 13C NMR spectrum of **14**

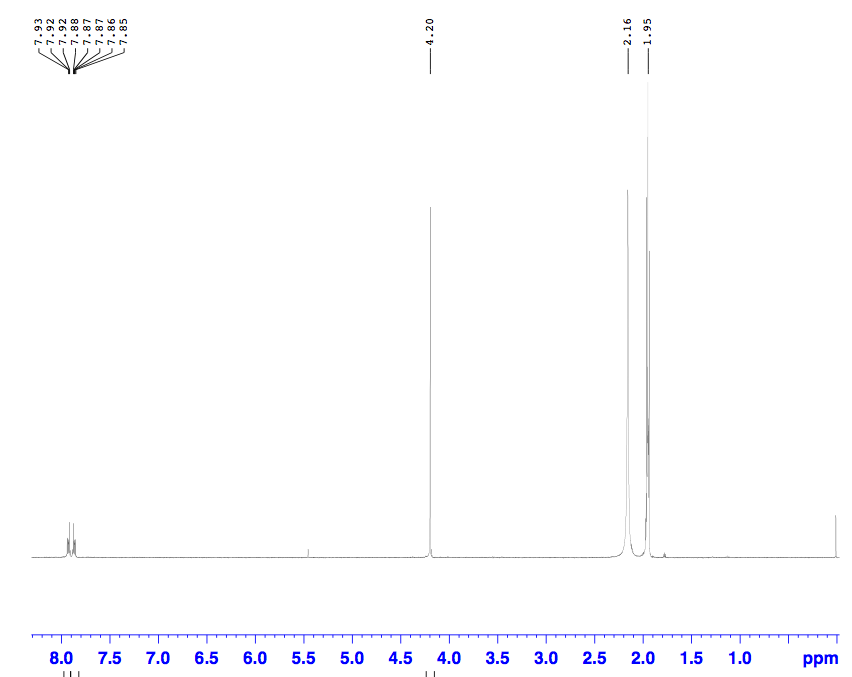


Figure S3. 1H NMR spectrum of compound **17**.

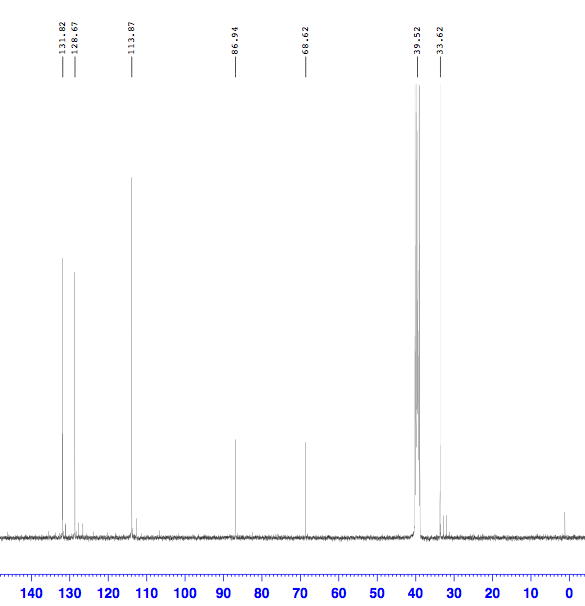
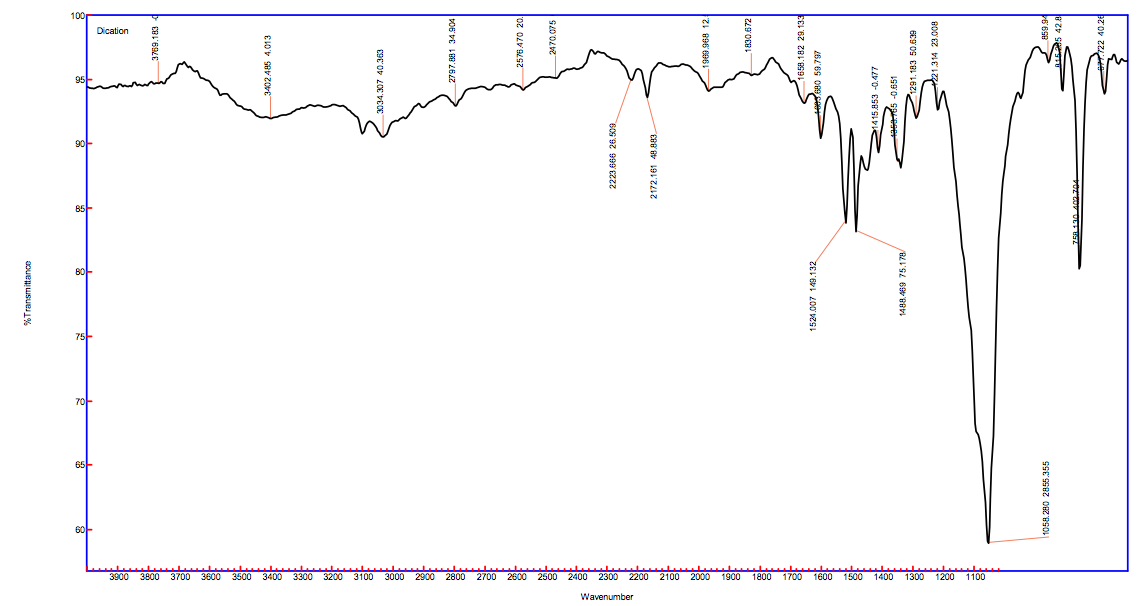


Figure S4. 13C NMR of compound **17**.



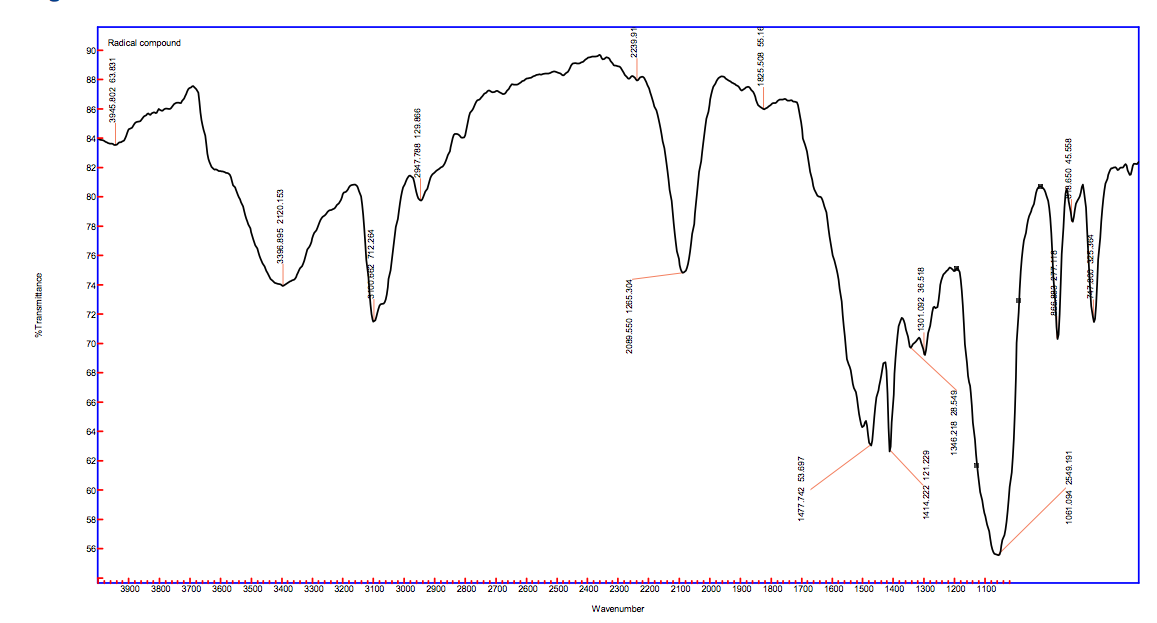


Figure S5. FT-IR spectra of compound **17** (top) and after reduction giving radical species hypothesized to be **18** (bottom).

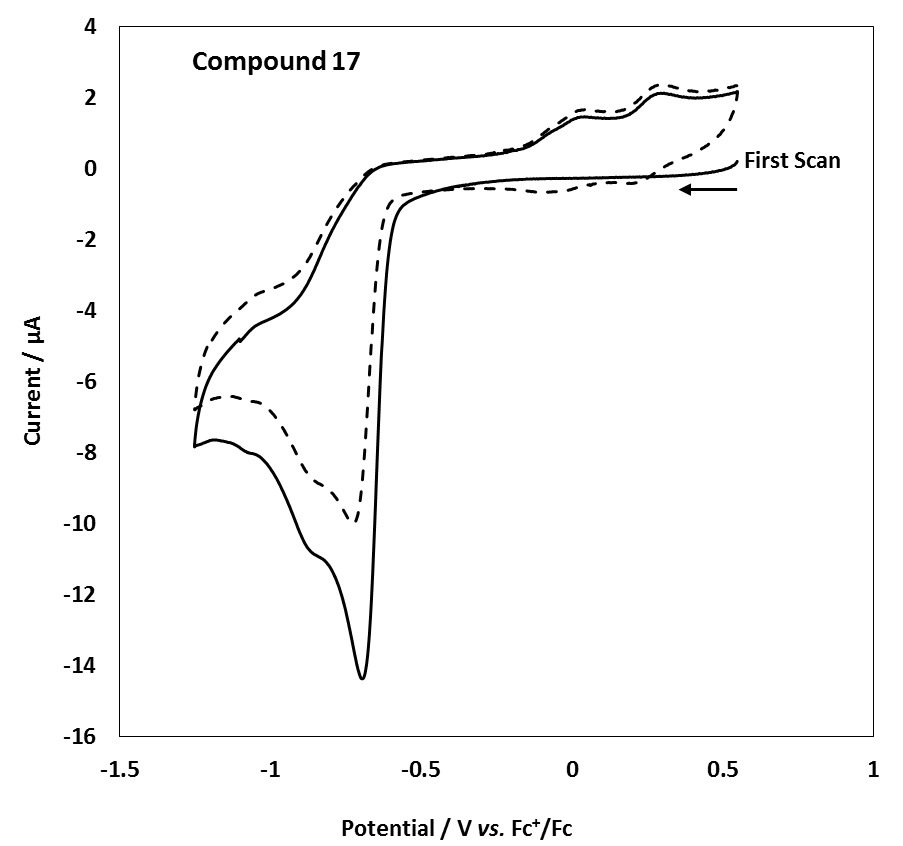


Figure S6. Cyclic voltammogram of a 1 mM solution of compound **17** using a3 mm glassy carbon disc electrode dissolved in acetonitrile containing 0.1 M TBAPF6 at a scan rate of 0.1 V/s. (The dashed-lines shows the second cycle of the voltammogram).

Coordinates and Energy for **[17]2+**

B3LYP Electronic Energy: -1068.82353496 Hartree

C 0.00000000 0.00000000 0.00000000

N -0.45853700 1.27939000 -0.54833800

C -1.78507000 1.64856600 -0.70752900

C -1.78513800 2.94608100 -1.26054900

N -0.45863300 3.31532800 -1.41985800

C 0.32848000 2.29738900 -0.98415300

C 1.73009900 2.29742100 -0.98416000

C 2.95297200 2.29737300 -0.98415300

C 4.30844800 2.29731700 -0.98413700

C 5.53131500 2.29729300 -0.98414900

C 6.93293400 2.29731400 -0.98412700

N 7.71995500 3.31528500 -0.54827800

C 9.04649000 2.94611600 -0.70750100

C 9.04655000 1.64861700 -1.26055400

N 7.72004100 1.27937700 -1.41986600

C 7.26160000 0.00004100 -1.96844100

H 7.61026100 -0.81530800 -1.32975900

H 6.17282800 -0.00261400 -2.00353400

H 7.65978700 -0.12321300 -2.97848200

C 10.2366410 0.97098300 -1.54849000

C 11.4143150 1.64604700 -1.26127000

C 11.4142610 2.94872500 -0.70645200

C 10.2365350 3.62376900 -0.41940100

H 10.2441930 4.62169300 0.00482000

H 12.3639150 3.43155400 -0.50069600

H 12.3640090 1.16324100 -1.46689600

H 10.2443720 -0.02692300 -1.97275200

C 7.26142700 4.59469200 0.00003500

H 7.60863700 5.40988300 -0.63964700

H 6.17270100 4.59662100 0.03671400

H 7.66093500 4.71884600 1.00943800

C -0.00019100 4.59462500 -1.96853200

H 1.08861300 4.59771500 -2.00256000

H -0.39747000 4.71735800 -2.97899700

H -0.34978500 5.41006100 -1.33047600

C -2.97522900 3.62372800 -1.54845200

C -4.15290300 2.94867100 -1.26121200

C -4.15284300 1.64598500 -0.70641200

C -2.97511600 0.97092600 -0.41940500

H -2.98277600 -0.02700400 0.00480600

H -5.10249500 1.16316100 -0.50063400

H -5.10259700 3.43148600 -1.46681400

H -2.98296000 4.62163000 -1.97272300

H 1.08874000 -0.00210500 0.03624400

H -0.39913400 -0.12395000 1.00957800

H -0.34758900 -0.81522700 -0.63942900

Coordinates and Energy for **[18]+**

B3LYP Electronic Energy: -1069.10780841 Hartree

C 0.00000000 0.00000000 0.00000000

N -0.45693100 -1.38108300 0.00007100

C -1.78603200 -1.78960200 0.00015900

C -1.78604900 -3.19700900 0.00020400

N -0.45695800 -3.60556000 0.00014400

C 0.35487700 -2.49333200 0.00006200

C 1.72512600 -2.49334800 -0.00002000

C 2.96944700 -2.49336000 -0.00009400

C 4.29695100 -2.49336200 0.00003000

C 5.54127200 -2.49337400 -0.00004400

C 6.91152100 -2.49339000 -0.00012600

N 7.72332900 -3.60563900 -0.00013500

C 9.05243000 -3.19712000 -0.00022300

C 9.05244700 -1.78971300 -0.00026800

N 7.72335600 -1.38116200 -0.00020800

C 7.26645900 -0.00006700 -0.00024100

H 7.63130000 0.51667900 -0.89330000

H 6.17633400 0.00988900 -0.00018900

H 7.63138400 0.51673100 0.89275400

C 10.2398440 -1.06122800 -0.00033300

C 11.4298160 -1.79132200 -0.00035900

C 11.4297990 -3.19556900 -0.00031400

C 10.2398090 -3.92563400 -0.00024000

H 10.2442510 -5.01040900 -0.00020500

H 12.3757260 -3.72750700 -0.00033600

H 12.3757560 -1.25940800 -0.00041600

H 10.2443130 0.02354700 -0.00036800

C 7.26639800 -4.98672200 -0.00006400

H 7.63130200 -5.50347300 0.89294700

H 6.17627200 -4.99665100 -0.00003800

H 7.63123400 -5.50353200 -0.89310700

C -0.00006100 -4.98665500 0.00017700

H 1.09006400 -4.99661100 0.00012500

H -0.36490200 -5.50340100 0.89323600

H -0.36498600 -5.50345300 -0.89281800

C -2.97344600 -3.92549400 0.00026900

C -4.16341800 -3.19540000 0.00029500

C -4.16340100 -1.79115300 0.00025000

C -2.97341100 -1.06108800 0.00017600

H -2.97785300 0.02368700 0.00014100

H -5.10932800 -1.25921500 0.00027200

H -5.10935800 -3.72731400 0.00035200

H -2.97791500 -5.01026900 0.00030400

H 1.09012600 0.00992900 -0.00002600

H -0.36490400 0.51675100 -0.89301100

H -0.36483600 0.51681000 0.89304300

Coordinates and Energy for neutral NHC-C-C-C-C-NHC

B3LYP Electronic Energy: -1069.26485094

C 0.00000000 0.00000000 0.00000000

N -0.45005900 -1.37230900 0.00006100

C -1.77418300 -1.78565200 0.00012400

C -1.77418500 -3.19787900 0.00016900

N -0.45006200 -3.61122500 0.00013300

C 0.39773600 -2.49176900 0.00006400

C 1.73793000 -2.49177100 0.00001200

C 3.00526700 -2.49177100 -0.00003700

C 4.30964300 -2.49175900 -0.00009700

C 5.57698000 -2.49175900 -0.00014600

C 6.91717400 -2.49176100 -0.00019800

N 7.76496900 -3.61122100 -0.00019500

C 9.08909300 -3.19787800 -0.00025800

C 9.08909500 -1.78565100 -0.00030300

N 7.76497200 -1.37230500 -0.00026700

C 7.31491400 0.00000500 -0.00029100

H 7.67325400 0.52940600 -0.89210700

H 6.22366200 0.00760000 -0.00024700

H 7.67332600 0.52946300 0.89146200

C 10.2763740 -1.06584200 -0.00037300

C 11.4795950 -1.79481300 -0.00039500

C 11.4795950 -3.18871700 -0.00035000

C 10.2763730 -3.91768700 -0.00028100

H 10.2791430 -5.00321000 -0.00024600

H 12.4228610 -3.72726800 -0.00036900

H 12.4228620 -1.25626200 -0.00044900

H 10.2791450 0.01968100 -0.00040800

C 7.31491000 -4.98353000 -0.00013400

H 7.67331900 -5.51293200 0.89165600

H 6.22366000 -4.99112600 -0.00009400

H 7.67325600 -5.51299000 -0.89191300

C -0.00000400 -4.98353500 0.00015700

H 1.09124800 -4.99113000 0.00011300

H -0.35834400 -5.51293600 0.89197300

H -0.35841600 -5.51299300 -0.89159600

C -2.96146400 -3.91768800 0.00023900

C -4.16468500 -3.18871700 0.00026100

C -4.16468500 -1.79481300 0.00021600

C -2.96146300 -1.06584300 0.00014700

H -2.96423300 0.01968000 0.00011200

H -5.10795100 -1.25626200 0.00023500

H -5.10795200 -3.72726800 0.00031500

H -2.96423500 -5.00321100 0.00027400

H 1.09125000 0.00759600 -0.00004000

H -0.35840900 0.52940200 -0.89179000

H -0.35834600 0.52946000 0.89177900

Coordinates and Energy for Cp2Co

B3LYP Electronic Energy: -1769.71652434 Hartree

Co 0.00000000 0.00000000 0.00000000

C -1.75167900 0.97885600 -0.71123500

C -1.69915300 -0.39691000 -1.13780600

C -1.75692300 -1.23016200 0.01085800

C -1.69782300 -0.37642200 1.14506900

C -1.75252600 0.99136700 0.69495600

H -1.75206900 1.86641000 1.33181000

H -1.68272000 -0.69480600 2.18000000

H -1.74406900 -2.31185800 0.02045200

H -1.68472000 -0.73310100 -2.16708800

H -1.75138700 1.84255600 -1.36341100

C 1.74999600 -0.98017800 0.71467100

C 1.69994100 0.39703600 1.13709400

C 1.75928800 1.22654000 -0.01408500

C 1.69888200 0.36929400 -1.14573200

C 1.75164700 -0.99713000 -0.69136000

H 1.74933100 -1.87409000 -1.32556000

H 1.68494200 0.68455400 -2.18164000

H 1.74873800 2.30822300 -0.02719900

H 1.68611000 0.73646200 2.16531700

H 1.74747400 -1.84177500 1.36963000

Coordinates and Energy for [Cp2Co]+

B3LYP Electronic Energy: -1769.52932078

Co 0.00000000 0.00000000 0.00000000

C -1.64743700 0.43573900 1.13310400

C -1.64813500 1.21206700 -0.06419400

C -1.64811900 0.31308000 -1.17254600

C -1.64802000 -1.01882200 -0.66017300

C -1.64741700 -0.94302400 0.76487100

H -1.62037200 -1.78338200 1.44624800

H -1.62254800 -1.92654300 -1.24889800

H -1.62269800 0.59246800 -2.21779600

H -1.62216000 2.29245800 -0.12149200

H -1.62197800 0.82472200 2.14269400

C 1.64745400 -0.43651700 -1.13289500

C 1.64786100 -1.21218400 0.06486400

C 1.64816700 -0.31280700 1.17269000

C 1.64795200 1.01878500 0.65965100

C 1.64752400 0.94234400 -0.76532900

H 1.62144900 1.78256100 -1.44760100

H 1.62265900 1.92674700 1.24773700

H 1.62287400 -0.59117700 2.21827500

H 1.62200600 -2.29260100 0.12305200

H 1.62179400 -0.82537000 -2.14216900