Supplementary Material (ESI) for Green Chemistry
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ELECTRONIC SUPPLEMENTARY INFORMATION

CO_2, COS and CS_2 Adducts of N-Heterocyclic Olefin and Their Application as Organocatalysts for Carbon Dioxide Fixation

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1. Crystallography

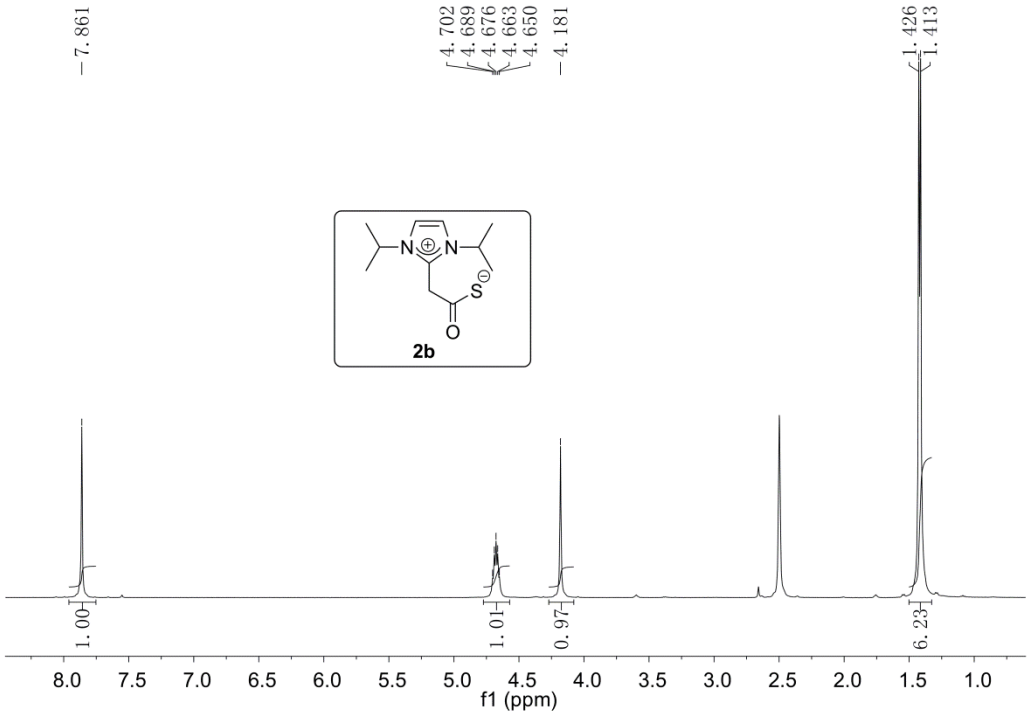
Single crystals of complexes **2b** and **2g** suitable for X-ray structural analysis were obtained from a CH_3CN/Et_2O solution at -30°C. Single crystals of complexes **2g** and **3g** suitable for X-ray structural analysis were obtained from a CH_2Cl_2/Et_2O solution at -30 °C. Diffraction datas were collected at 220 K on a Bruker SMART-CCD diffractometer using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods and refined by full-matrix least squares on F^2. All nonhydrogen atoms were refined anisotropically, and the hydrogen atoms were included in idealized positions. All calculations were performed using the SHELXTL crystallographic software packages. Details of the crystal data, data collections, and structure refinements are summarized in Table S1. CCDC-1062154 (**2b**), CCDC-1062155 (**2g**), CCDC-1062156 (**3b**) and CCDC-1062157 (**3g**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

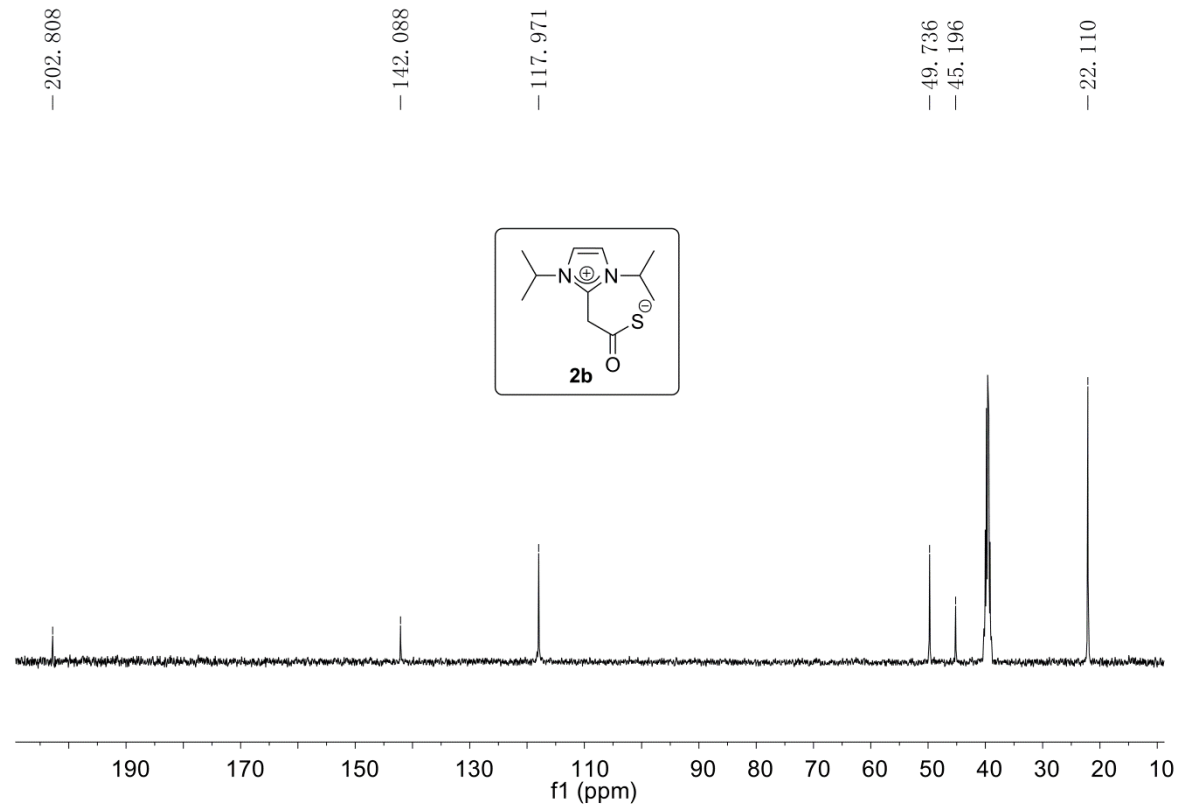
Table S1. Crystal data and structural refinement details for complexes **2b**, **2g, 3b and 3g**

	2b	**2g**	**3b**	**3g**
mol formula	$C_{11}H_{18}N_2OS$	$C_{20}H_{28}N_2OS$	$C_{11}H_{18}N_2S_2$	$C_{20}H_{28}N_2S_2$
molwt	226.30	344.50	242.39	360.56
crystsyst	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	P2(1)/n	P2(1)/c	P2(1)/n	P2(1)/c
a/Å	12.6450(3)	10.4317(3)	7.995(1)	10.167(1)
b/Å	15.1066(4)	15.4783(5)	15.115(2)	16.078(2)
c/Å	13.2140(2)	11.9638(4)	11.488(2)	12.986(1)
α/deg	90.00	90.00	90.00	90.00

β/deg	93.207(2)	102.189(2)	107.186(5)	103.802(5)
γ/deg	90.00	90.00	90.00	90.00
V/Å^3	2520.2(1)	1888.2(1)	1326.3(3)	2061.4(4)
R_{int}	0.0499	0.0471	0.0222	0.0257
R1 (I >2σ)	0.0546	0.0510	0.0464	0.0441
wR2 (I >2σ)	0.1051	0.1149	0.1201	0.1059
GOF	1.027	1.054	1.074	1.037

2, Representative ^{1}H NMR and ^{13}C NMR comparison for 2b, 2g, 3b and 3g.

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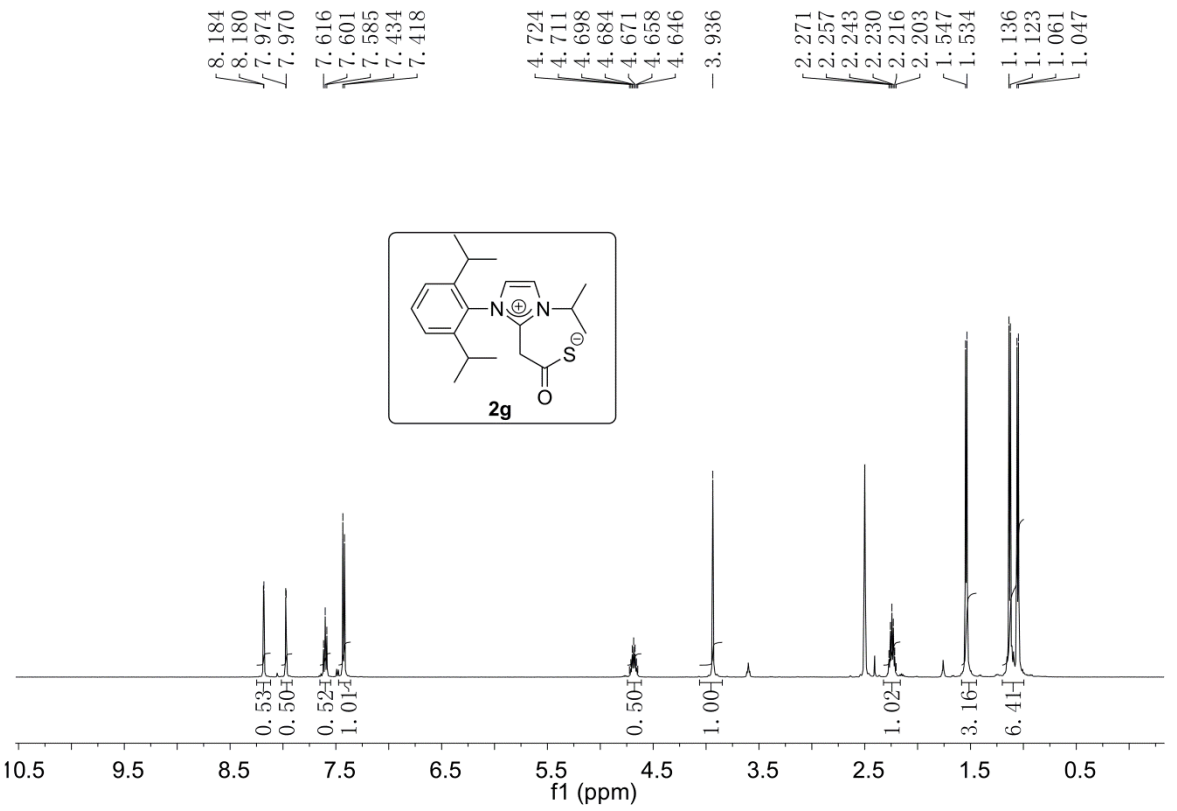
2b
190
170
150
130
110
90
80
70
60
50
40
30
20
10
f1 (ppm)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8.180
7.974
7.970
7.616
7.601
7.585
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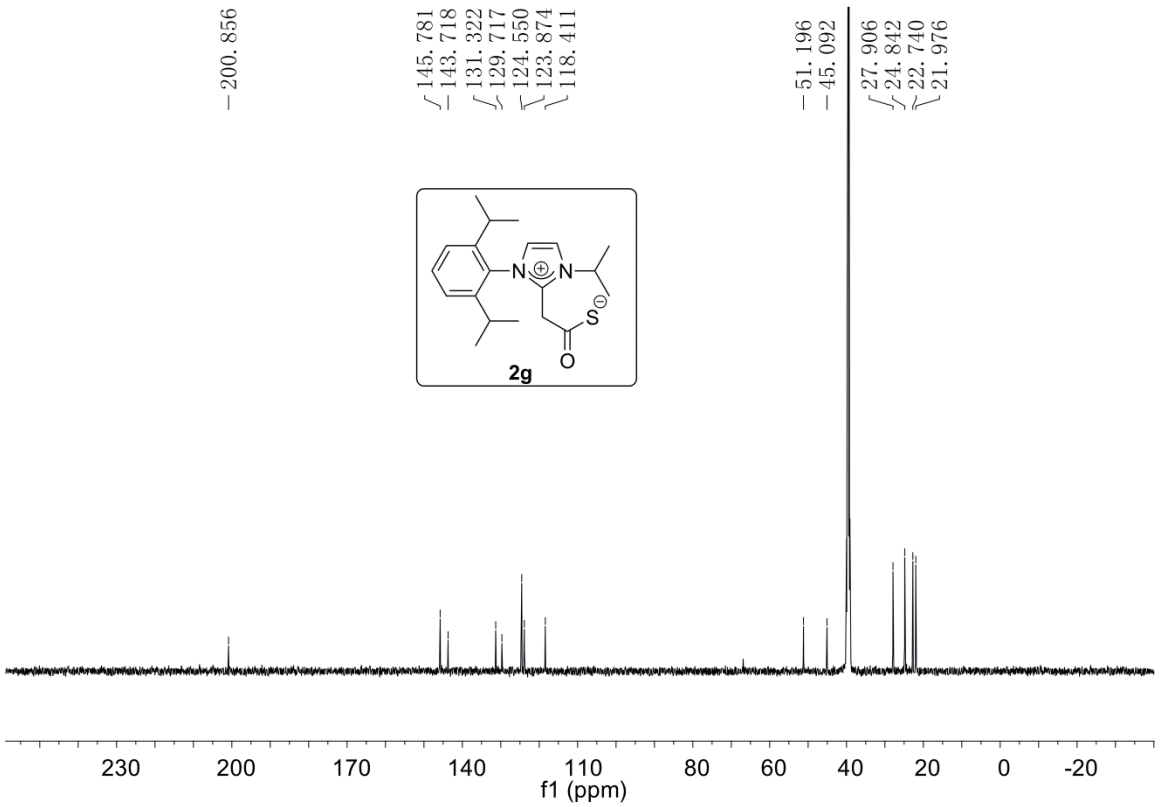
4.698
4.684
4.671
4.658
4.646
3.936
2.271
2.257
2.243
2.230
2.216
2.203
1.547
1.534
1.136
1.123
1.061
1.047
2g
0.53
0.50
0.52
1.01
0.50
1.00
1.02
3.16
6.41
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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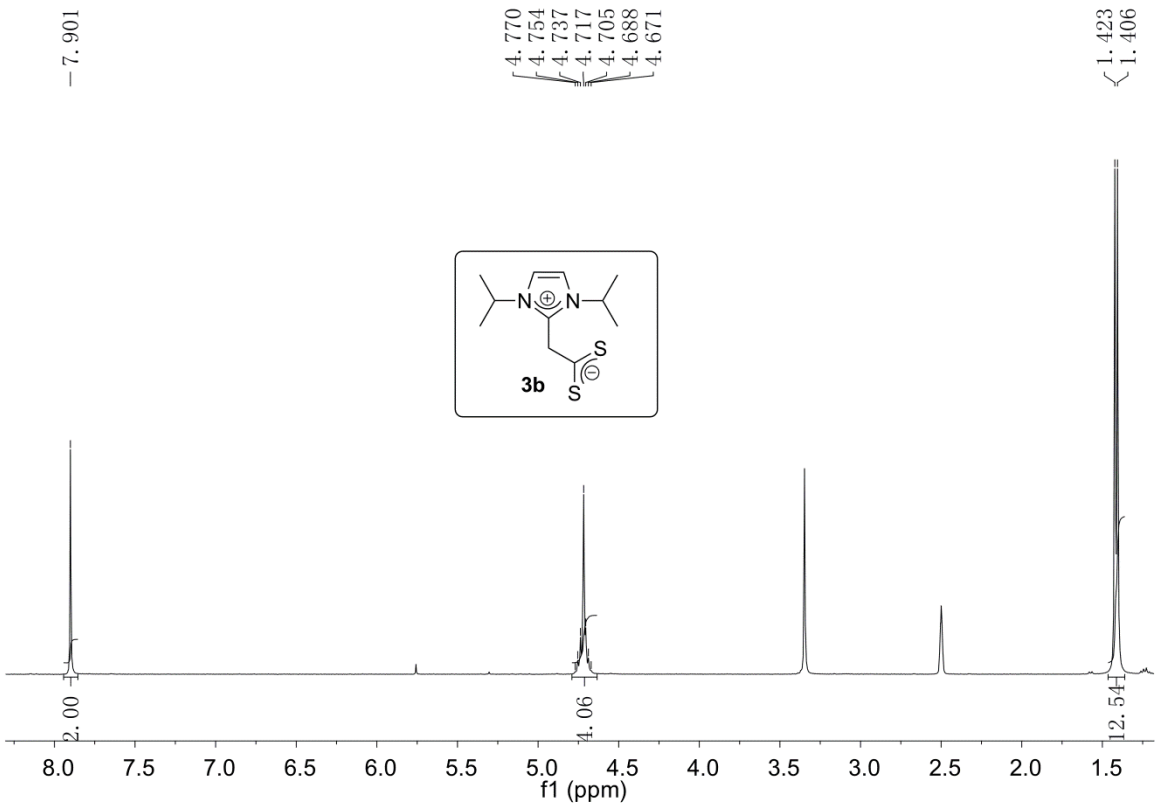
131.322
129.717
124.550
123.874
118.411
51.196
45.092
27.906
24.842
22.740
21.976
2g
230
200
170
140
110
80
60
40
20
0
-20
f1 (ppm)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4.737
4.717
4.705
4.688
4.671
1.423
1.406
3b
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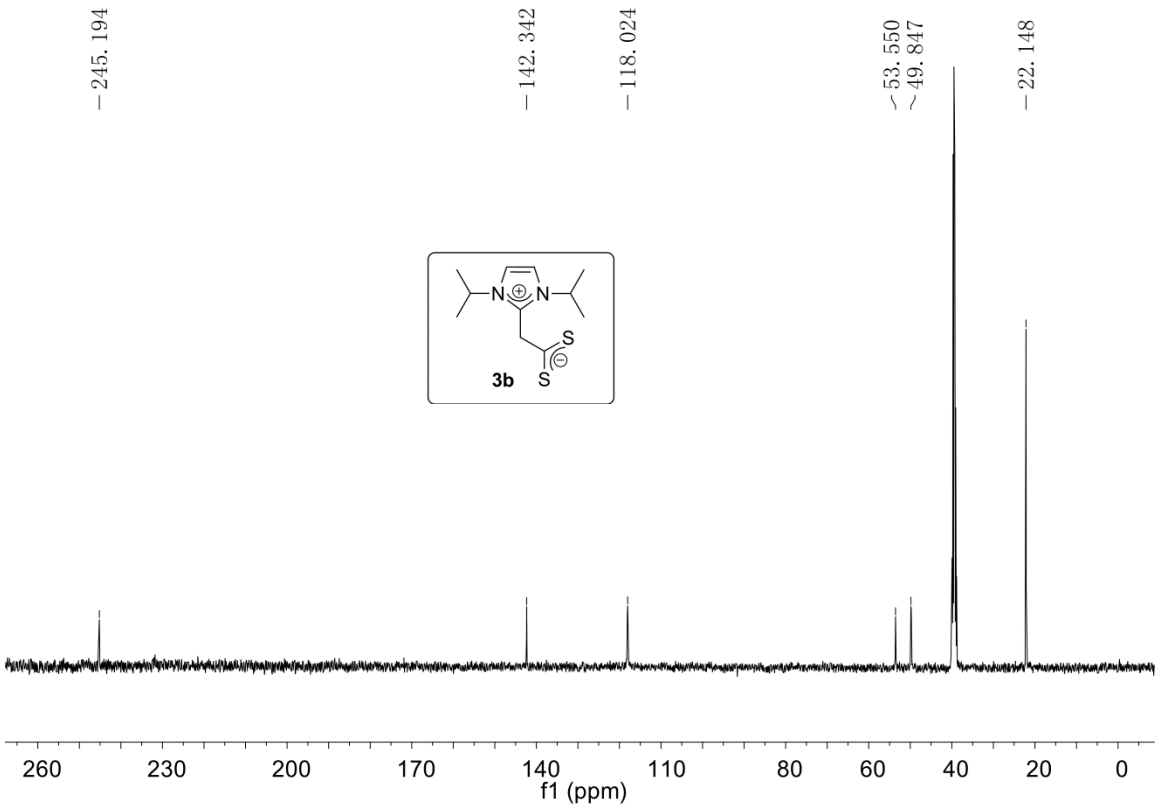
4.06
12.54
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)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80
60
40
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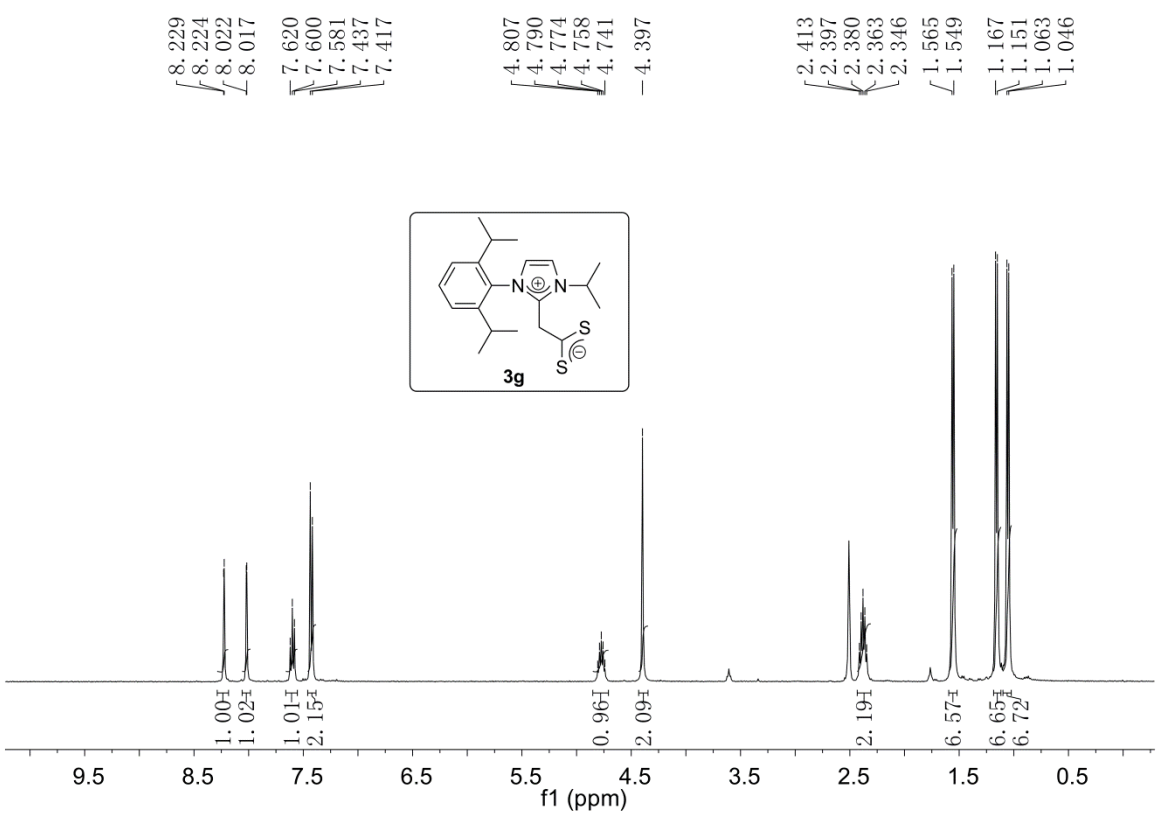
f1 (ppm)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7.620
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4.807
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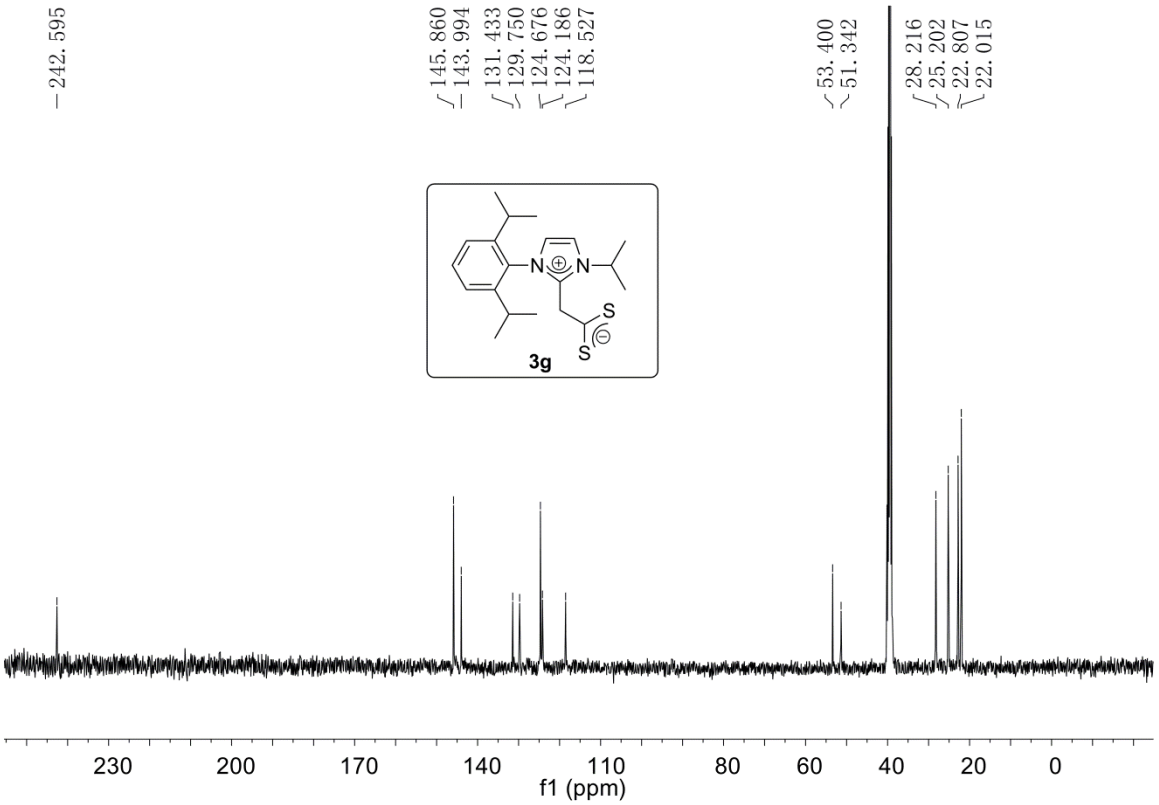
4.758
4.741
4.397
2.413
2.397
2.380
2.363
2.346
1.565
1.549
1.167
1.151
1.063
1.046
3g
1.00
1.02
1.01
2.15
0.96
2.09
2.19
6.57
6.65
6.72
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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143.994
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124.186
118.527
53.400
51.342
28.216
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22.807
22.015
3g
230
200
170
140
110
80
60
40
20
0
f1 (ppm)