Supporting Information for

Highly Effective Capture and Subsequent Catalytic Transformation of Low-concentration CO_2 by Superbasic Guanidines

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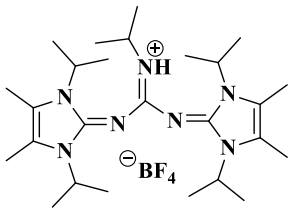
1. General procedures:

All manipulations of oxygen- and/or moisture-sensitive materials were performed under an atmosphere of dry nitrogen using standard Schlenk or dry box techniques. Solvents were dried by standard methods and distilled under argon. ^{1}H, and ^{13}C NMR spectra were recorded on Varian Inova 500, Varian Inova 400 and Bruker 600 spectrometers.

2. Synthesis of N′N′-Bis(imidazolylidene)guanidinium tetrafluoroborates (BIG salts 1a-1d). The BIG salts were prepared according to a modified literature procedure[S1]:

A Schlenk flask was charged with the 2-chloroimidazolium salt (1.0 equiv.), anhydrous KF (8.0 equiv.) and the corresponding guanidinium salt (0.5 equiv.) in CH_3CN solution. Then, the resulting suspension was stirred at 60 ^{o}C for the indicated period of time. After the reaction finished, the solid residues were filtered and the filtrate was transferred into a separation funnel. A diluted aq. solution of $NaBF_4$ was added to the solution followed by vigorous shaking. Then the organic phase was separated and extracted with $CHCl_3$. The combined organic fractions were dried by anhydrous Na_2SO_4. After removed the volatiles under vacuum, the residue was purified by column chromatography (SiO_2, CH_2Cl_2/CH_3OH=40:1) to give the desired products.

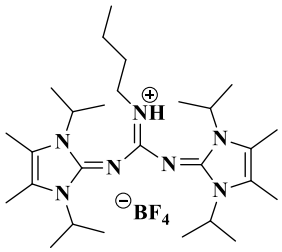
BIG salt 1a: Prepared from amino(isopropylamino)methaniminium iodide (2.5 mmol), 2-chloroimidazolium salt (5.0 mmol), KF (40.0 mmol), CH_3CN (10 mL) following the general procedure. BIG salt **1a** was isolated as a white solid. Yield 56%.



^{1}H NMR (500 MHz, $CDCl_3$) δ 4.62 – 4.40 (m, 4H), 4.06 (dd, *J* = 12.8, 6.3 Hz, 2H), 2.21 (s, 12H), 1.45 (d, *J* = 7.0 Hz, 24H), 1.18 (d, *J* = 6.0 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 156.8, 147.8, 120.5, 48.0, 44.3, 23.0, 21.4, 10.1. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values.[S1]

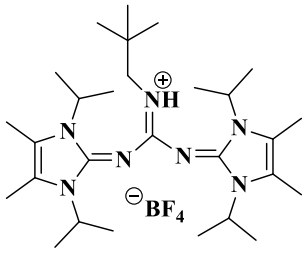
BIG salt 1b: Prepared from amino(butylamino)methaniminium iodide (2.5 mmol), 2-

chloroimidazolium salt (5.0 mmol), KF (40.0 mmol), CH_3CN (10 mL) following the general procedure. BIG salt **1b** was isolated as a white solid. Yield 73%.



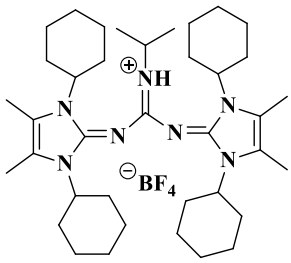
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.44 (dt, *J* = 13.6, 6.7 Hz, 4H), 4.23 (s, 1H), 3.25 (dd, *J* = 13.2, 6.5 Hz, 2H), 2.16 (s, 12H), 1.49 (dd, *J* = 14.1, 7.7 Hz, 2H), 1.40 (d, *J* = 7.0 Hz, 24H), 1.28 (td, *J* = 14.5, 7.2 Hz, 2H), 0.85 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 157.3, 147.7, 120.1, 47.8, 42.3, 32.2, 21.1, 20.0, 13.8, 9.8. **IR**: 3205, 2972, 2927, 1541, 1486, 1425, 1057. **HRMS (ESI)**: m/z calculated for $[C_{27}H_{50}N_7]^+$ $(M)^+$ 472.4122, found 472.4111.

BIG salt 1c: Prepared from amino(neopentylamino)methaniminium iodide (2.5 mmol), 2-chloroimidazolium salt (5.0 mmol), KF (40.0 mmol), CH_3CN (10 mL) following the general procedure. BIG salt **1c** was isolated as a white solid. Yield 50%.



^{1}H NMR (400 MHz, $CDCl_3$) δ 4.58 – 4.44 (m, 4H), 4.31 (t, J = 5.9 Hz, 1H), 3.21 (d, J = 6.2 Hz, 1H), 2.22 (s, 12H), 1.46 (d, J = 7.1 Hz, 24H), 0.91 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.7, 147.7, 120.4, 53.8, 48.0, 32.4, 27.5, 21.4, 10.1. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values. [S1]

BIG salt 1d: Prepared from amino(isopropylamino)methaniminium iodide (2.5 mmol), 2-chloroimidazolium salt(5.0 mmol), KF(40.0 mmol), CH_3CN (10 mL) following the general procedure. BIG salt **1d** was isolated as a white solid. Yield 48%.



^{1}H NMR (400 MHz, $CDCl_3$) δ 4.37 – 3.94 (m, 6H), 2.25 (s, 12H), 1.89 (d, *J* = 8.0 Hz, 24H), 1.72 (d, *J* = 12.6 Hz, 4H), 1.50 – 1.02 (m, 18H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.8, 148.0, 120.7, 56.8, 44.3, 31.0, 26.3, 25.2, 23.3, 10.8. All the resonances in ^{1}H and ^{13}C NMR spectra were in good agreement with literature values. [S1]

3. TGA analysis of BIGs-CO_2 adducts

The thermal stability of BIG-CO_2 adducts (**3a-3d**) was studied by means of thermogravimetric analysis (TGA). The experimental temperature rose from 30 ºC to 600 ºC under N_2 atmosphere. Ramp rate = 5 °C/min.

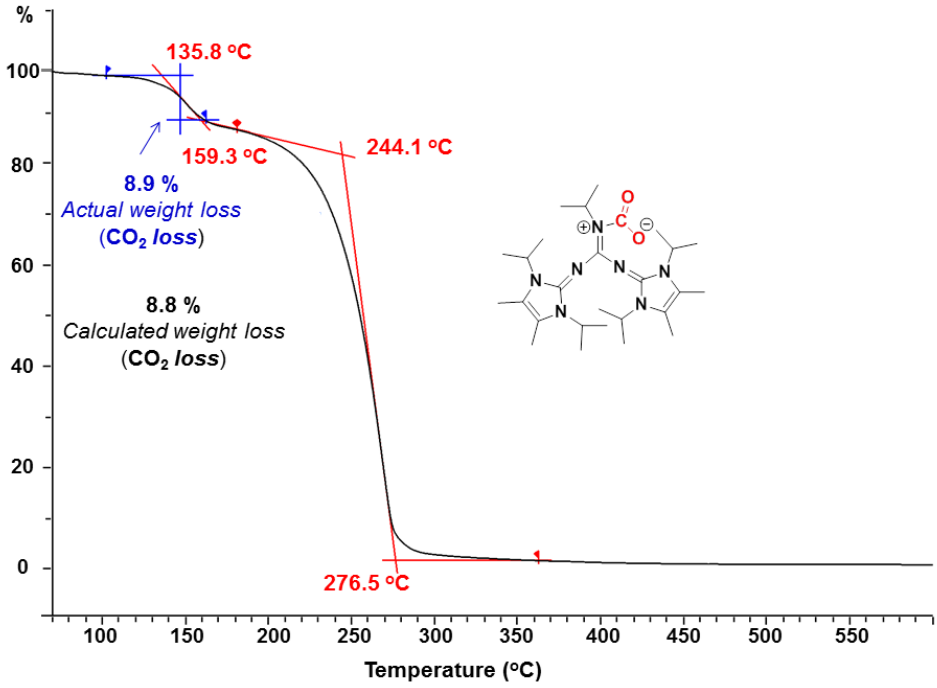


Figure S1. TGA of BIG-CO_2 adduct **3a** under N_2 atmosphere. Ramp rate = 5 °C/min

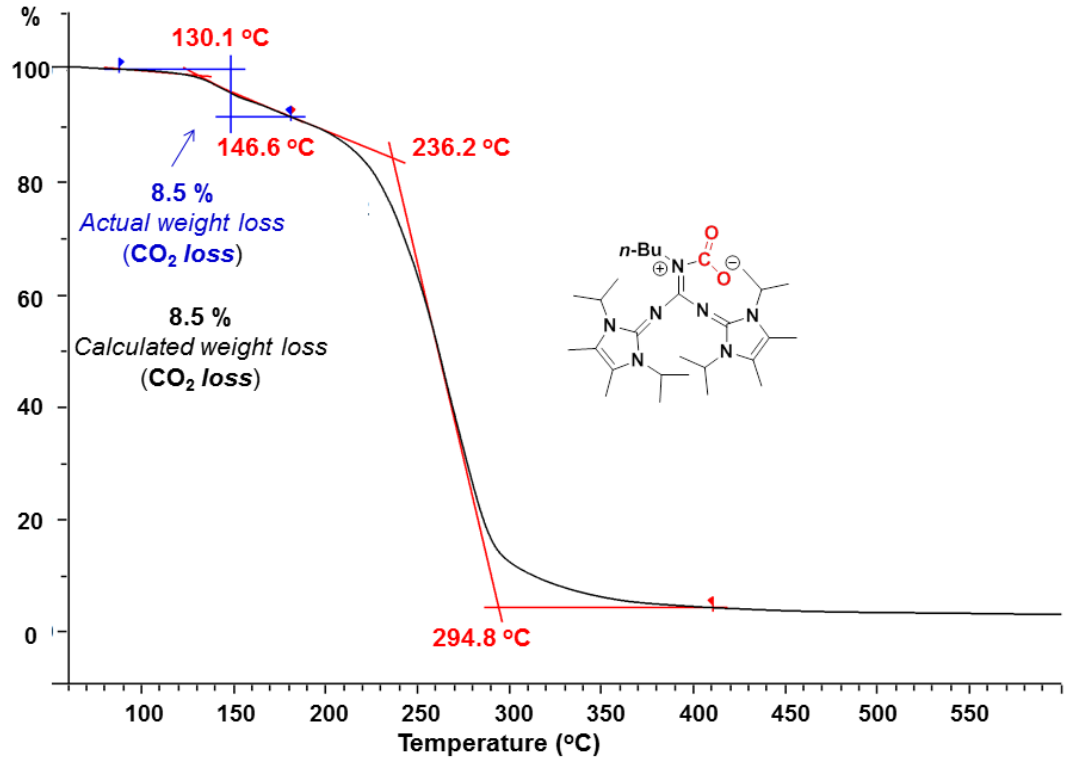


Figure S2. TGA of BIG-CO_2 adduct **3b** under N_2 atmosphere. Ramp rate = 5 °C/min

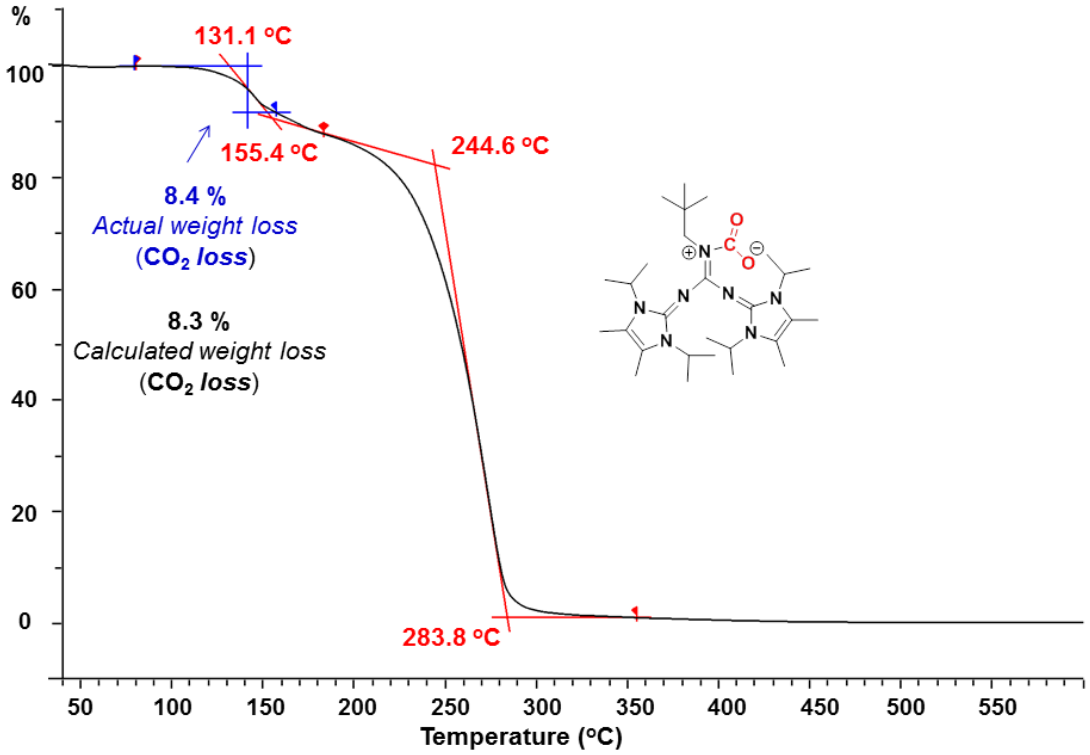


Figure S3. TGA of BIG-CO_2 adduct **3c** under N_2 atmosphere. Ramp rate = 5 °C/min

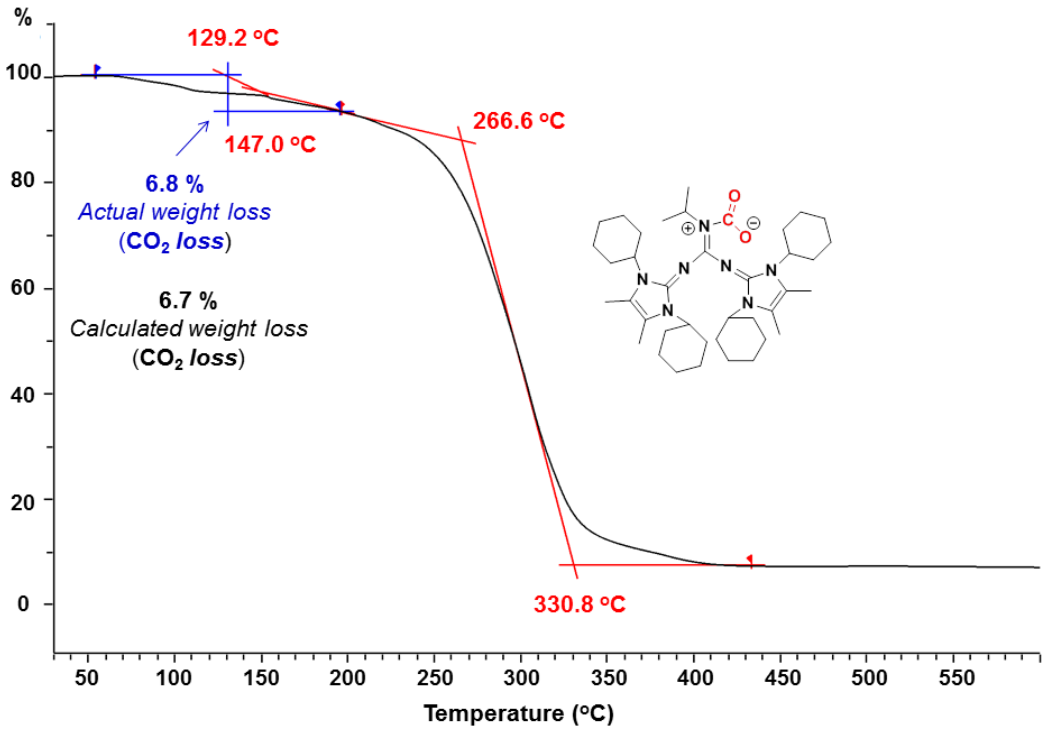


Figure S4. TGA of BIG-CO_2 adduct **3d** under N_2 atmosphere. Ramp rate = 5 °C/min

4. DFT calculation for reversible capture and release of CO_2 by BIG bases

In order to illustrate the ability of **BIG** bases for reversible capture and release of CO_2, DFT calculation was performed with Gaussian 16. [S2] All geometries of **BIG** bases, TS, and BIG-CO_2 adducts were fully optimized at the M06-2X/def2-SVP level of theory. Intrinsic reaction coordinates (IRC) were calculated for all of the transition states to confirm that the structures indeed connect two relevant minima. To improve the accuracy of the energy, the single-point energy of each optimized structure was calculated at the M06-2X (SMD, *n*-hexane)/def2-TZVP level.

As shown in Figure S5, only the formation **3d** from **2d** with CO_2 is endergonic by 2.4 kcal/mol, and the energy barrier for the nucleophilic activation process is 9.7 kcal/mol. By contrast, the formations of **3a-3c** are obviously exergonic with lower energy barriers (4.4-7.6 kcal/mol). Moreover, we also investigated the reversible CO_2 release behavior of BIG-CO_2 adducts, and the corresponding energy barriers are the range of 7.3-8.6 kcal/mol, suggesting that it is feasible to release CO_2 under high temperature conditions.

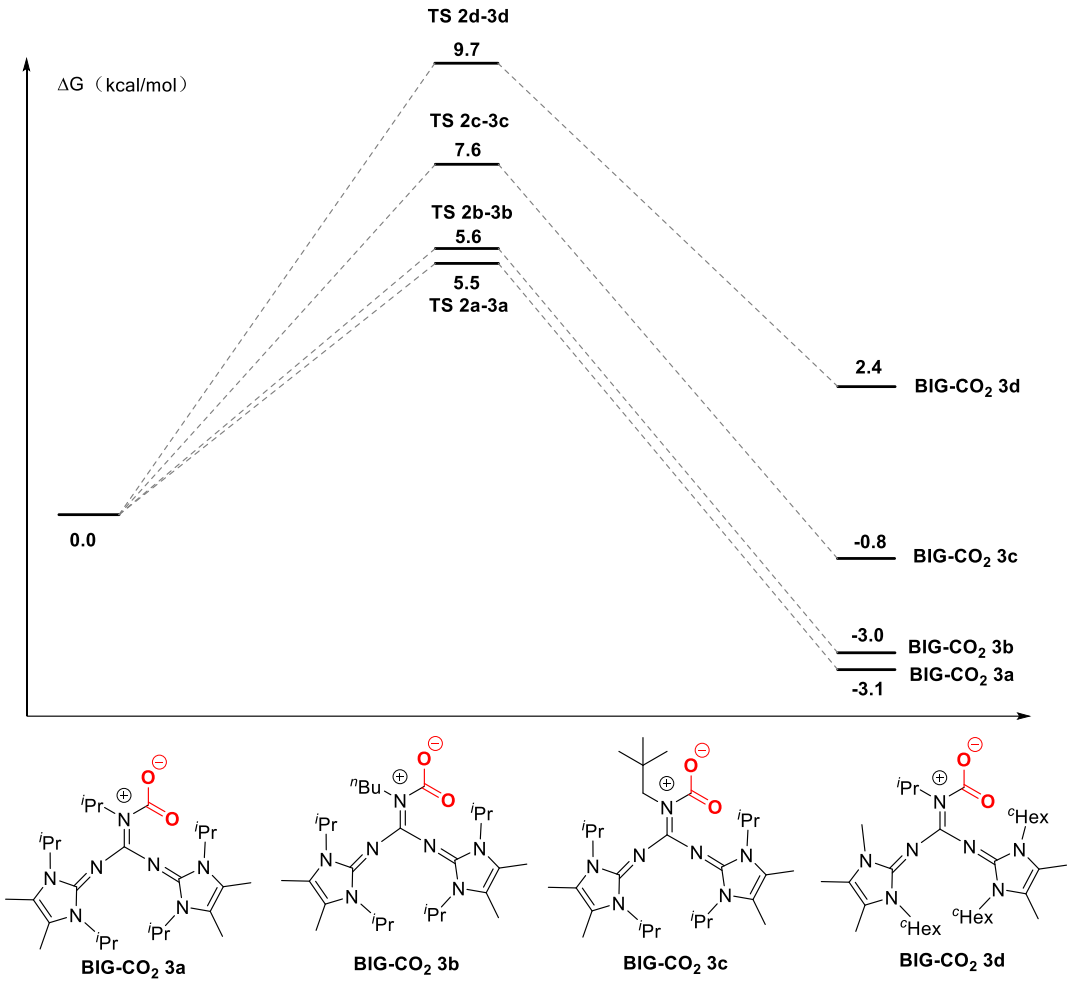
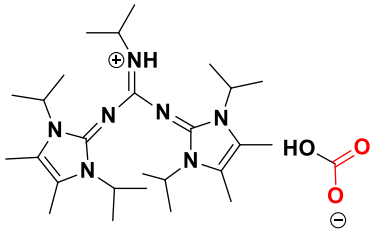


Figure S5. Computed Gibbs free energy profile for the reversible CO_2 capture and release ability of **BIG** bases

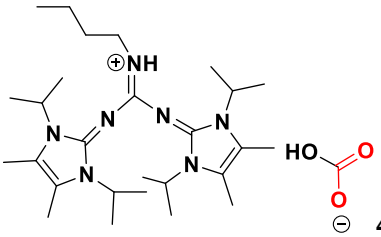
5. Protonation of BIG-CO_2 adducts in the presence of H_2O

A 10 mL vial was charged successively with BIG-CO_2 (0.5 mmol), H_2O (1.0 mmol) and THF (1.0 mL), then the reaction mixture was stirred for 2 hours under room temperature. After removal of the solvent, the residue was purified by column chromatography (SiO_2, CH_2Cl_2:CH_3OH = 20:1) to give the desired product as colorless solid.

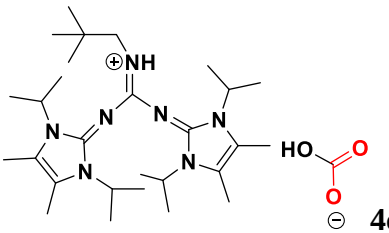


4a (Yield: 95%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.69 – 4.28 (m, 4H), 4.19 – 3.85 (m, 1H), 2.19 (s, 12H), 1.42 (d, *J* = 7.1 Hz, 24H), 1.16 (d, *J*

= 6.5 Hz, 6H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.3, 156.4, 147.7, 120.3, 48.0, 44.0, 23.2, 21.4, 10.1. **IR**: 2981, 2926, 1648, 1582, 1542, 1474. **HRMS (ESI)**: m/z calculated for $[C_{26}H_{48}N_7]^+$ $(M)^+$ 458.3966, found 458.3962.



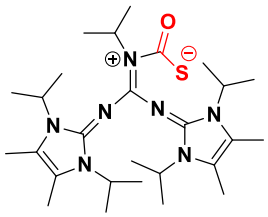
4b (Yield: 92%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.42 – 4.48 (m, 4H), 3.21 (t, *J* = 7.5 Hz, 2H), 2.16 (s, 12H), 1.23-1.49 (m, 4H), 1.39 (d, *J* = 7.4 Hz, 24H), 0.84 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.5, 157.6, 148.0, 120.1, 47.8, 42.2, 32.5, 21.2, 20.2, 13.9, 10.0. **IR**: 2966, 2929, 2156, 1487, 1180, 1075. **HRMS (ESI)**: m/z calculated for $[C_{27}H_{50}N_7]^+$ $(M)^+$ 472.4122, found 472.4126.



4c (Yield: 90%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.46 – 4.55 (m, 4H), 3.20 (s, 2H), 2.24 (s, 12 H), 1.46 (d, *J* = 7.1 Hz, 24H), 0.91 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 158.4, 157.6, 147.7, 120.3, 53.6, 47.9, 32.3, 27.5, 21.3, 10.0. **IR**: 2958, 1642, 1541, 1486, 1423, 1340, 1204, 1106. **HRMS (ESI)**: m/z calculated for $[C_{28}H_{52}N_7]^+$ $(M)^+$ 486.4279, found 486.4287.

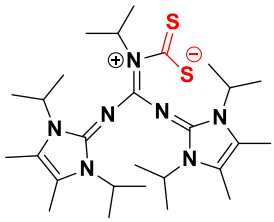
6. Synthesis of BIG-COS adducts 5 and BIG-CS_2 6

In a glove box, BIG salts **1a** (545 mg, 1.0 mmol) was added to a suspension of KHMDS (199 mg, 1.0 mmol) in THF (10 mL) and the mixture was stirred at 25 ^{o}C for 2 h. The solvent was removed *in vacuo* and the residue was extracted by *n*-hexane (10 mL). After filtration to remove the resulting inorganic salt, the filtrate was exposed to 1.0 atm of COS at room temperature for 2 h. The resulting precipitate was collected *via* filtration, washed with *n*-hexane (3×5 mL) and then dried *in vacuo* to afford BIG-COS adduct **5** as a white solid (501 mg, 97% yield).



^{1}H NMR (400 MHz, CD_3CN) δ 4.62 – 4.29 (m, 4H), 4.33 – 3.96 (m, 1H), 2.20 (s, 12H), 1.41 (d, *J* = 7.1 Hz, 24H), 1.14 (d, *J* = 6.6 Hz, 6H). **^{13}C NMR** (101 MHz, CD_3CN)) δ 202.3, 157.4, 148.8, 121.1, 48.8, 44.7, 23.3, 21.4, 10.1. **IR**: 2972, 2942, 1650, 1542, 1511, 1476. **HRMS (ESI)**: calcd for $C_{27}H_{47}N_7OS$: 458.3966 [M-COS+H]$^+$. Found: 458.3959 [M-COS+H]$^+$.

In a glove box, BIG salts **1a** (545 mg, 1.0 mmol) was added to a suspension of KHMDS (199 mg, 1.0 mmol) in THF (10 mL) and the mixture was stirred at ambient temperature for 2 h. The solvent was removed *in vacuo* and the residue was extracted by *n*-hexane (10 mL). After filtration to remove the resulting inorganic salt, CS_2 (152 mg, 2 mmol) was added. The solution was stirred to room temperature for 2 h. The precipitate was formed and collected *via* filtration. Subsequent the solid was washed with *n*-hexane (3×5 mL) to afford the BIG-CS_2 adduct **6** in 98% yield as yellow solid.



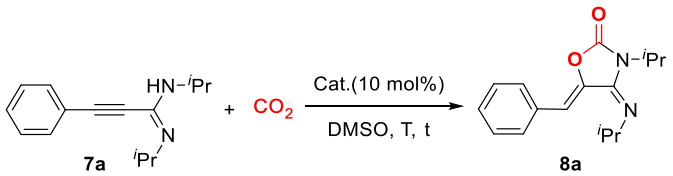
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.10 – 5.75 (m, 1H), 5.34 – 4.87 (m, 4H), 2.18 (s, 12H), 1.41 (d, *J* = 6.8 Hz, 30H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 221.6, 157.6, 146.6, 120.0, 55.61, 48.4, 21.2, 20.4, 10.1. **IR**: 2972, 2925, 1654, 1585, 1465, 1083. **HRMS (ESI)**: calcd for $C_{27}H_{47}N_7S_2$: 534.3407 [M+H]$^+$. Found: 534.3399[M+H]$^+$.

7. General Procedure for the cyclization reaction of propiolamidines with CO_2

Initially, we began our studies using the *N*,*N'*-diisopropyl-3-phenylpropiolimidamide **7a** as the model substrate for this process. The results are shown in **Table S1**. When using 10 mol% BIG-CO_2 addcuts **3a** as organocatalyst, the yield of **8a** was 47% in 1.0 atm of pure CO_2 under 80 ^{o}C within 4 hours (entry 1). Under the same conditions, **3b** presented the highest catalytic activity, affording **8a** in 65% (entry 2). In order to investigate the catalyst performance under practical conditions, a

mixture gas containing 0.15 bar CO_2 and 0.85 bar N_2 to simulate flue gas from the power plant was employed for the cycloaddition reaction. By further using 10% CO_2, the desired product **8a** was produced in lower yield (entries 5-8), indicating that the CO_2 concentration have an important influence on the catalytic activity. Further optimization of the reaction conditions showed that the reaction time has a profound impact on the efficiency of this reaction and a better yield of 90% was obtained for 24 h (entry 10). It is important to emphasize that the reaction could also carry out under dry air atmosphere (entry 11), affording **5a** in 25% yield with prolonging the reaction time and increasing the catalyst loading. Notably, the reduced temperature has negative effects on the yield (entry 12). As expected, control experiments revealed no products formation in the absence of catalyst (entry 13).

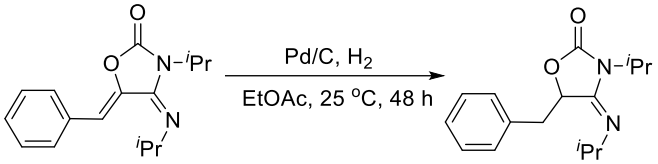
Table S1. Reaction of CO_2 with **7a** catalyzed by BIG-CO_2 adducts



entry	Cat.	CO_2 concentration (%)	t (h)	Yield [b] (%)
1	**3a**	100	4	47
2	**3b**	100	4	65
3	**3c**	100	4	38
4	**3d**	100	4	40
5 [c]	**3a**	10	4	30
6 [c]	**3b**	10	4	36
7 [c]	**3c**	10	4	25
8 [c]	**3d**	10	4	26
9 [c]	**3b**	10	12	74
10 [c]	**3b**	10	24	90
11 [d]	**3b**	**Air**	**72**	**25**
12 [e]	**3b**	100	24	<5%
13 [f]	**-**	100	24	0

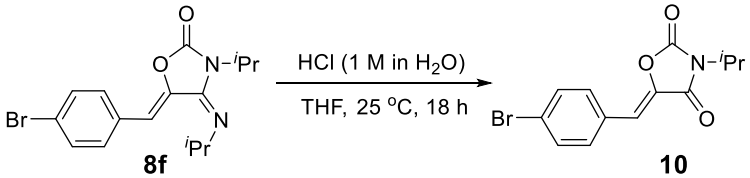
[a] General reaction conditions: **7a** (0.25 mmol), **cat.** (0.025 mmol), CO_2 balloon, 80 °C, DMSO (1.0 mL). [b] Determined by ^{1}H NMR using 1,3,5-Trimethoxybenzene as an internal standard [c] Balloon (10% CO_2, 90% N_2), [d] Under dry air atmosphere, cat. 30%. [e] 25 °C. [f] No cat.

8. General Procedure for Further Transformations



8a **9**

A 20 mL autoclave containing a stir bar was charged with **8a** (0.5 mmol), 10% Pd/C (6 mg) and 2.0 mL EtOAc. The autoclave was pressurized into H_2 (2.0 MPa). After the reaction mixture was stirred at room temperature for 48 h, the solution filtered and concentrated under vacuum. The residue was then purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to give product **7** as white solid (98% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 3H), 7.21 (s, 2H), 5.21 (s, 1H), 4.09 (d, *J* = 6.4 Hz, 1H), 3.73 (d, *J* = 5.5 Hz, 1H), 3.22 (d, *J* = 14.6 Hz, 1H), 3.00 (d, *J* = 14.6 Hz, 1H), 1.32 (s, 3H), 1.15 (d, *J* = 14.6 Hz, 6H), 1.01 (s, 3H).^{13}C NMR (151 MHz, $CDCl_3$) δ 155.4, 151.6, 133.6, 130.0, 128.7, 127.7, 74.7, 49.8, 44.1, 38.7, 24.9, 24.6, 18.5. IR: 2972, 2912, 2845, 1780, 1689, 1407, 1385, 1243, 1138, 1079, 1034, 764, 743, 698. HRMS (ESI): calcd for $C_{16}H_{22}N_2O_2$: 275.1754 $[M+H]^+$. Found: 275.1745 $[M+H]^+$.



8f **10**

To a solution of **5f** (0.5 mmol) in THF (5.0 mL) was slowly added HCl (1M in H_2O, 2 mL). Then the mixture was stirred at room temperature for 18 h. The reaction solution was concentrated under vacuum. The residue was then purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 30:1) to give product **6** as white solid (98% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.7 Hz, 2H), 7.56 (d, *J* = 7.8 Hz, 2H), 6.65 (s, 1H), 4.63 – 4.11 (m, 1H), 1.49 (d, *J* = 6.7 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.3, 151.5, 137.9, 132.6, 132.5, 130.0, 125.1, 111.8, 45.7, 19.7.IR: 2987, 2920, 1814, 1741, 1722, 1668, 1489, 1410, 1370, 1248, 1076, 895, 822, 763. HRMS (ESI): calcd for $C_{13}H_{12}BrNO_3$: 310.0073 $[M+H]^+$. Found: 310.0074

$[M+H]^+$.

9. Crystallography

Diffraction data 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 [S3] and refined by full-matrix least squares on F2. All nonhydrogen atoms were refined anisotropically, and the hydrogen atoms were included in idealized positions. All calculations were performed using the SHELXTL[S4] crystallographic software packages. CCDC 1997581 (**3b**), CCDC 1997583 (**4a**), CCDC 1997582 (**6**), CCDC 1997584 (**8a**), CCDC 1997585 (**8g**) 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.

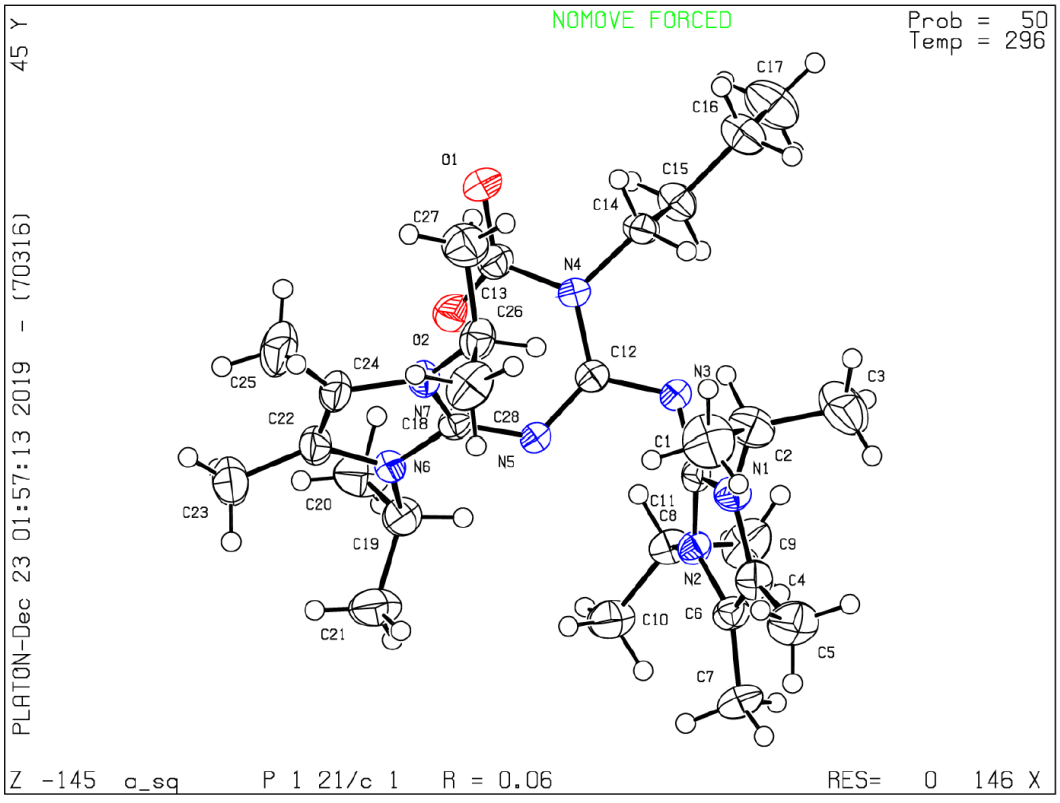


Figure S6. ORTEP Single Crystal X-Ray Diffraction of **3b**

Table S2. Crystal data and structure refinement for **3b**

```
Bond precision:   C-C = 0.0044 A          Wavelength=0.71073

Cell:             a=12.003(7)      b=19.823(11)       c=16.309(9)
                  alpha=90         beta=111.5900      gamma=90
Temperature:      296 K

                 Calculated                 Reported
Volume           3608(4)                    3608(4)
Space group      P 21/c                     P 1 21/c 1
Hall group       -P 2ybc                    -P 2ybc
Moiety formula   C28 H49 N7 O2 [+ solvent]  C28 H49 N7 O2
Sum formula      C28 H49 N7 O2 [+ solvent]  C28 H49 N7 O2
Mr               515.74                     515.74
Dx,g cm-3        0.950                      0.949
Z                4                          4
Mu (mm-1)        0.062                      0.062
F000             1128.0                     1128.0
F000'            1128.37
h,k,lmax         14,24,20                   14,24,20
Nref             7102                       6015
Tmin,Tmax        0.987,0.994                0.505,0.746
Tmin'            0.987

Correction method= # Reported T Limits: Tmin=0.505 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.847           Theta(max)= 26.021

R(reflections)= 0.0574( 2624)      wR2(reflections)= 0.1506( 6015)

S = 0.787                  Npar= 347
```

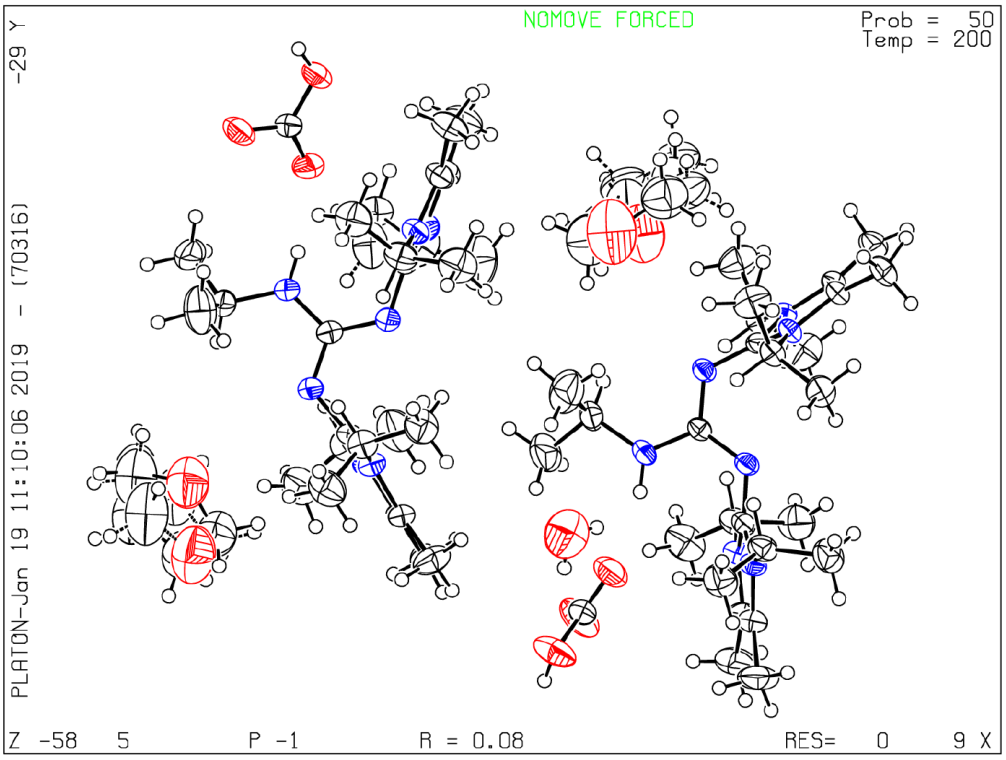


Figure S7. ORTEP Single Crystal X-Ray Diffraction of **4a**

Table S3. Crystal data and structure refinement for **4a**

Bond precision: C-C = 0.0051 A Wavelength=0.71073

Cell: a=12.8442(7) b=17.5019(9) c=18.6407(9)
alpha=63.996(1) beta=70.836(1) gamma=69.475(1)
Temperature: 200 K

	Calculated	Reported
Volume	3450.4(3)	3450.4(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H47 N7, C26 H48 N7, 2(C4 H8 O), 2(C H O3), H2 O	2(C H O3), C26 H48 N7, C26 H47 N7, H2 O, 2(C4 H8 O)
Sum formula	C62 H115 N14 O9	C62 H115 N14 O9
Mr	1200.68	1200.67
Dx,g cm-3	1.156	1.156
Z	2	2
Mu (mm-1)	0.078	0.078
F000	1314.0	1314.0
F000'	1314.50	
h,k,lmax	15,21,22	15,21,22
Nref	12850	12780
Tmin,Tmax	0.989,0.992	0.605,0.746
Tmin'	0.988	

Correction method= # Reported T Limits: Tmin=0.605 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.498

R(reflections)= 0.0793(9588) wR2(reflections)= 0.2485(12780)

S = 1.041 Npar= 859

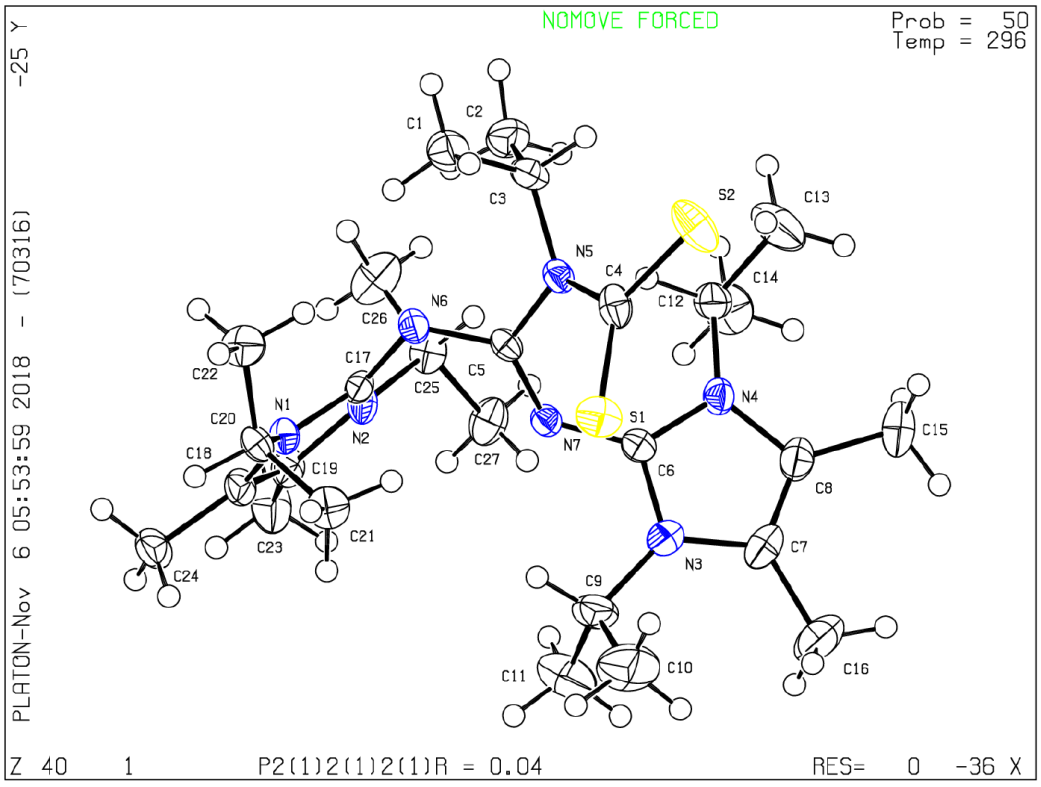


Figure S8. ORTEP Single Crystal X-Ray Diffraction of **6**

Table S4. Crystal data and structure refinement for **6**

```
Bond precision:  C-C = 0.0040 A          Wavelength=0.71073

Cell:            a=11.9503(6)     b=12.9375(6)     c=19.6351(10)
                 alpha=90         beta=90          gamma=90
Temperature:     296 K

                 Calculated                Reported
Volume           3035.7(3)                 3035.7(3)
Space group      P 21 21 21                P2(1)2(1)2(
Hall group       P 2ac 2ab                 ?
Moiety formula   C27 H47 N7 S2             ?
Sum formula      C27 H47 N7 S2             C27 H47 N7 S2
Mr               533.84                    533.84
Dx,g cm-3        1.168                     1.168
Z                4                         4
Mu (mm-1)        0.203                     0.203
F000             1160.0                    1160.0
F000'            1161.28
h,k,lmax         14,15,23                  14,15,23
Nref             5351[ 3020]               5351
Tmin,Tmax        0.971,0.980               0.673,0.746
Tmin'            0.968

Correction method= # Reported T Limits: Tmin=0.673 Tmax=0.746
AbsCorr = MULTI SCAN

Data completeness= 1.77/1.00      Theta(max)= 25.000

R(reflections)= 0.0407( 4537)     wR2(reflections)= 0.1016( 5351)

S = 1.048                 Npar= 325
```

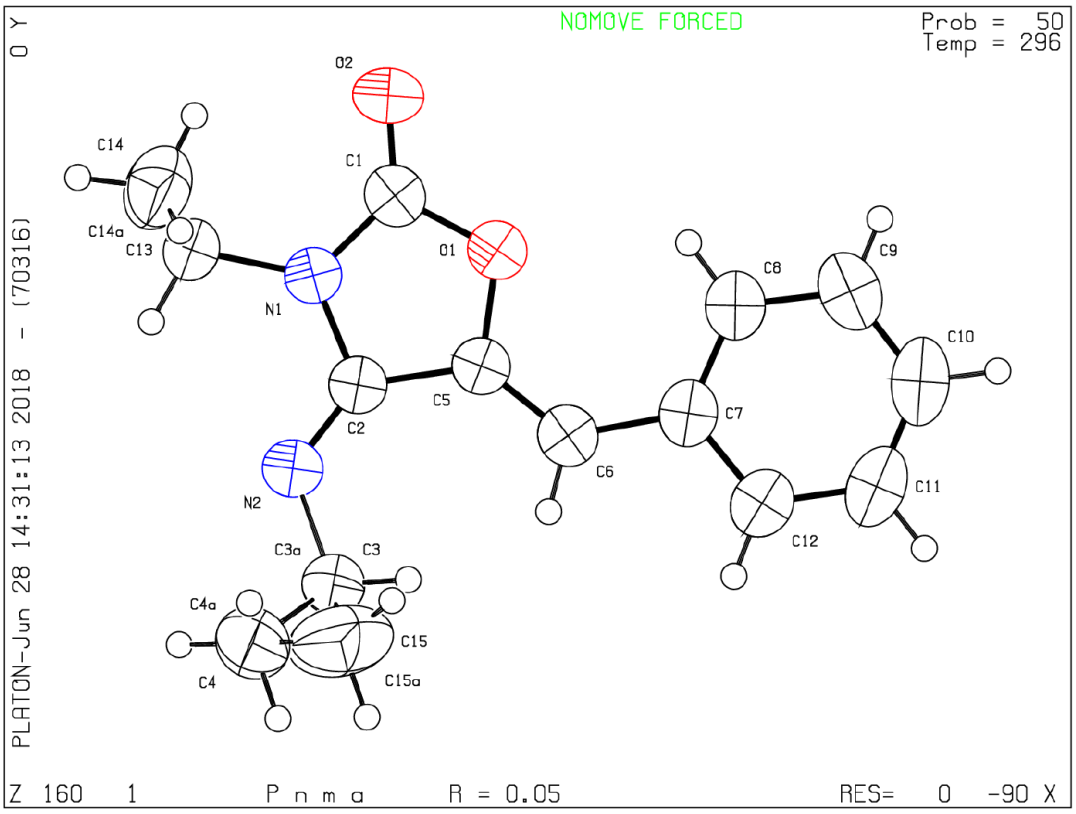


Figure S9. ORTEP Single Crystal X-Ray Diffraction of **8a**

Table S5. Crystal data and structure refinement for **8a**

Bond precision: C-C = 0.0035 A		Wavelength=0.71073	
Cell:	a=12.863(4)	b=7.173(2)	c=16.464(5)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	1519.1(8)	1519.1(8)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C16 H20 N2 O2	C16 H20 N2 O2
Sum formula	C16 H20 N2 O2	C16 H20 N2 O2
Mr	272.34	272.34
Dx,g cm-3	1.191	1.191
Z	4	4
Mu (mm-1)	0.079	0.079
F000	584.0	584.0
F000'	584.24	
h,k,lmax	16,9,21	16,9,21
Nref	1887	1877
Tmin,Tmax		0.612,0.746
Tmin'		

Correction method= # Reported T Limits: Tmin=0.612 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.498

R(reflections)= 0.0472(983) wR2(reflections)= 0.1486(1877)

S = 1.024 Npar= 131

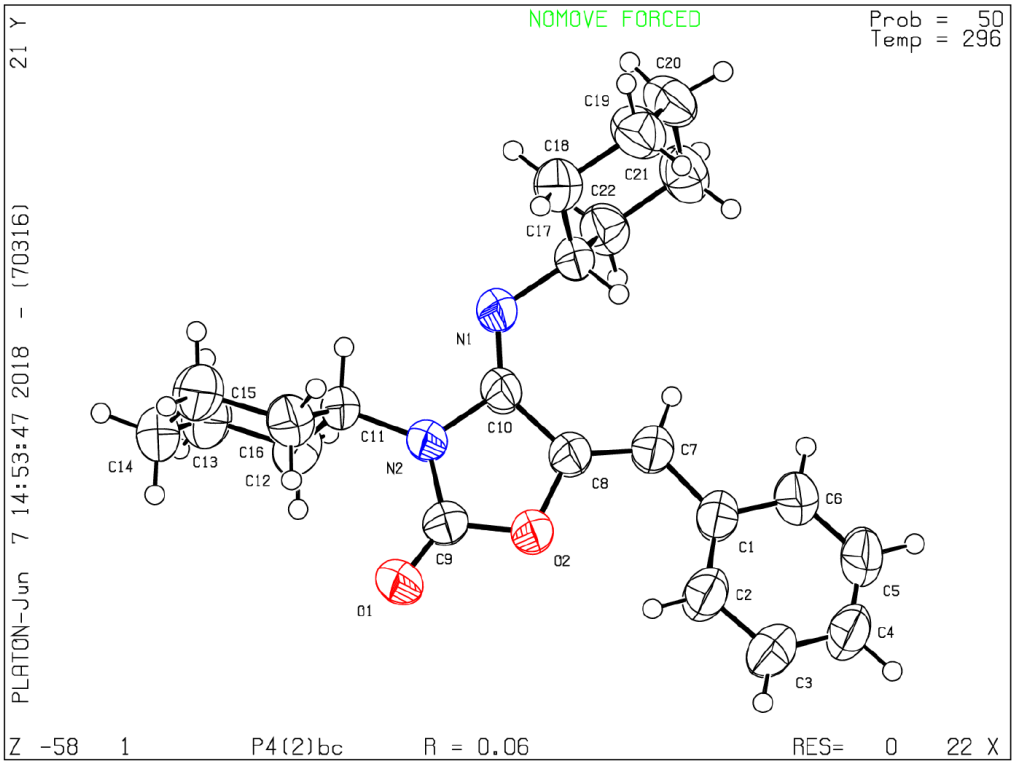


Figure S10. ORTEP Single Crystal X-Ray Diffraction of **8g**

Table S6. Crystal data and structure refinement for **8g**

Bond precision:	C-C = 0.0052 A	Wavelength=0.71073	
Cell:	a=20.029(3)	b=20.029(3)	c=9.929(3)
	alpha=90	beta=90	gamma=90
Temperature:	296 K		

	Calculated	Reported
Volume	3983.1(17)	3983.3(15)
Space group	P 42 b c	P4(2)bc
Hall group	P 4c -2ab	?
Moiety formula	C22 H28 N2 O2	?
Sum formula	C22 H28 N2 O2	C22 H28 N2 O2
Mr	352.46	352.46
Dx,g cm-3	1.176	1.175
Z	8	8
Mu (mm-1)	0.075	0.075
F000	1520.0	1520.0
F000'	1520.60	
h,k,lmax	26,26,12	26,26,12
Nref	4607[2442]	4571
Tmin,Tmax	0.989,0.993	0.527,0.746
Tmin'	0.988	

Correction method= # Reported T Limits: Tmin=0.527 Tmax=0.746
AbsCorr = MULTI SCAN

Data completeness= 1.87/0.99 Theta(max)= 27.580

R(reflections)= 0.0577(2273) wR2(reflections)= 0.1664(4571)

S = 1.001 Npar= 235

10. Reference

[S1] Vazdar, K.; Kunetskiy, R.; Saame, J.; Kaupmees, K.; Leito, I.; Jahn, U., *Angew. Chem., Int. Ed.* **2014,** *53,* 1435-1438.

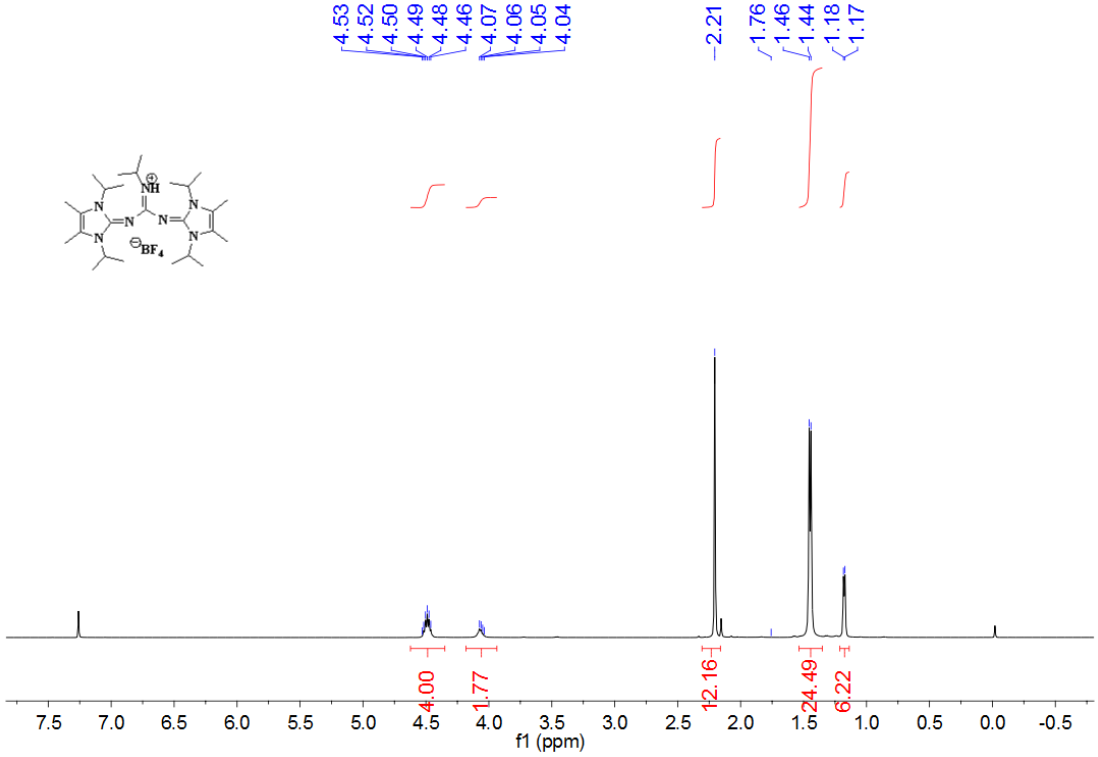
[S2] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J.

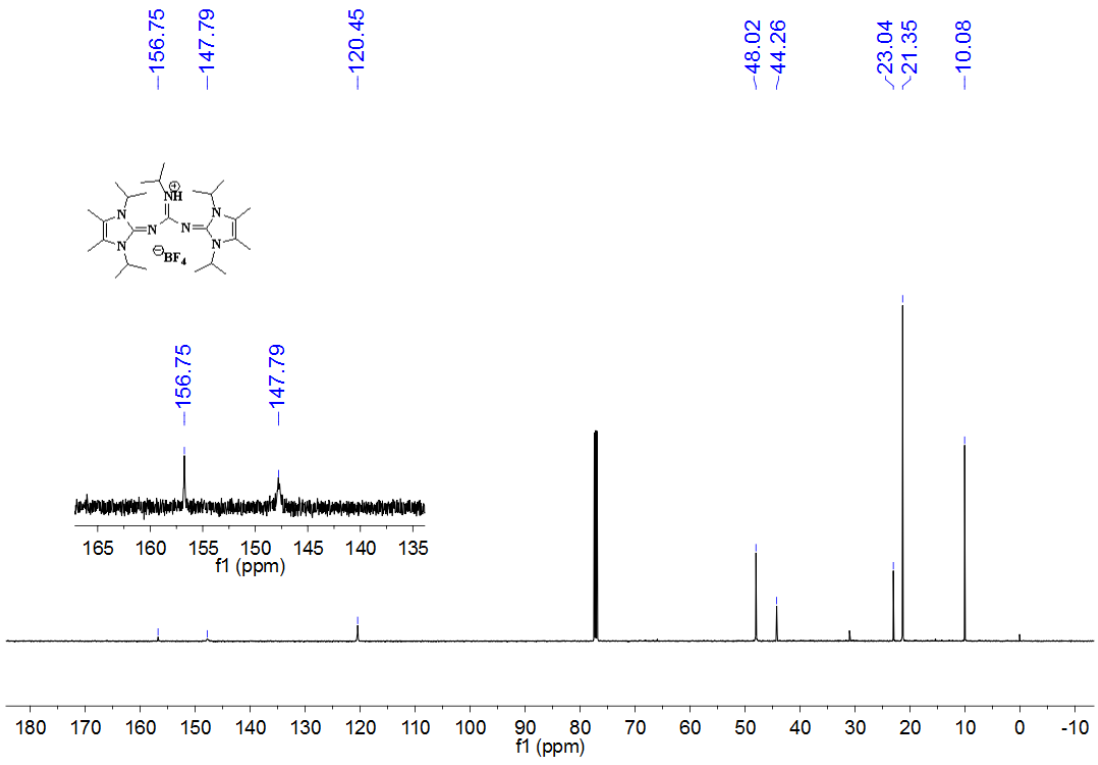
B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.

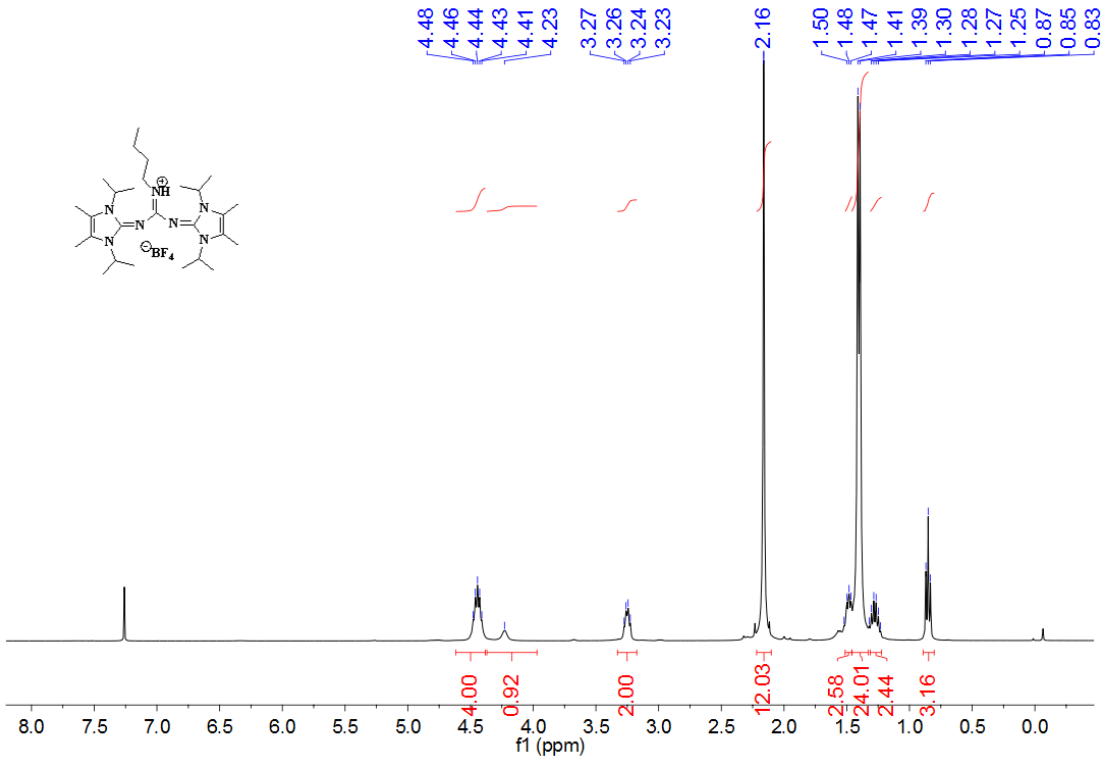
[S3] SHELXTL PC; Siemens Analytical X-ray Instruments, Madison, WI, 1993.

[S4] Sheldrick, G. M. SHELXTL Structure Determination Programs, version 5.0, PC; Siemens Analytical Systems, Madison, WI, 1994.

11. NMR spectra



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1.48
1.47
1.41
1.39
1.30
1.28
1.27
1.25
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2.00
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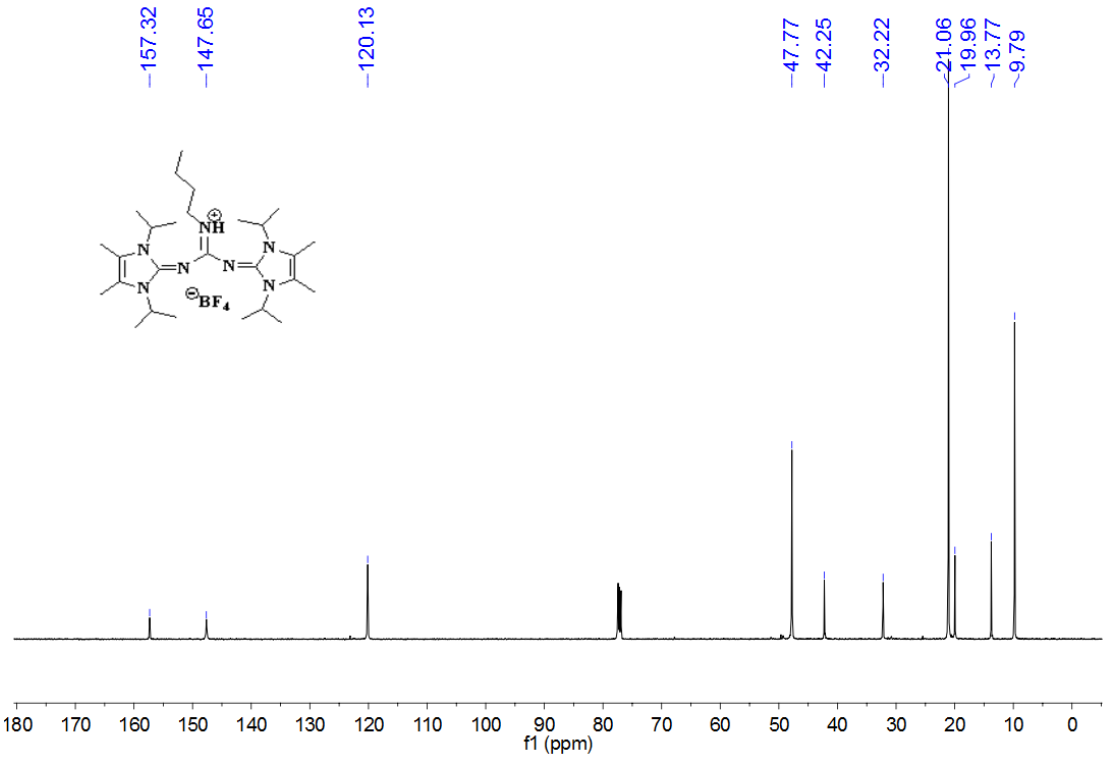
24.01
2.44
3.16
f1 (ppm)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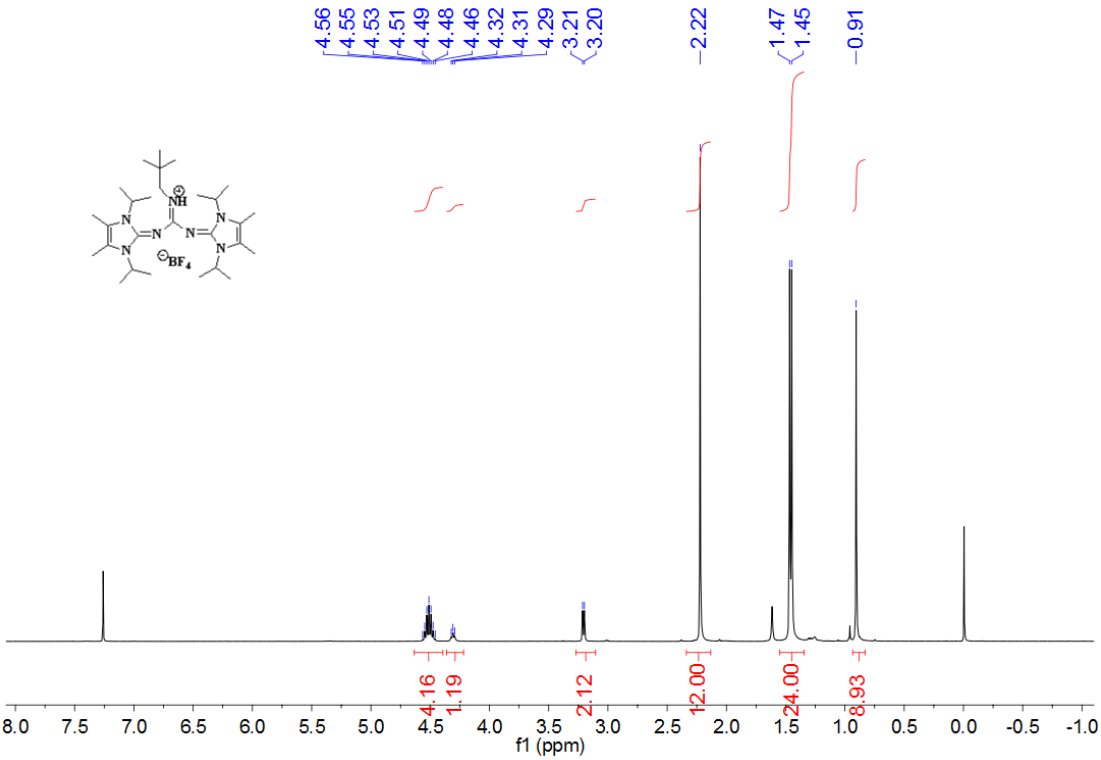
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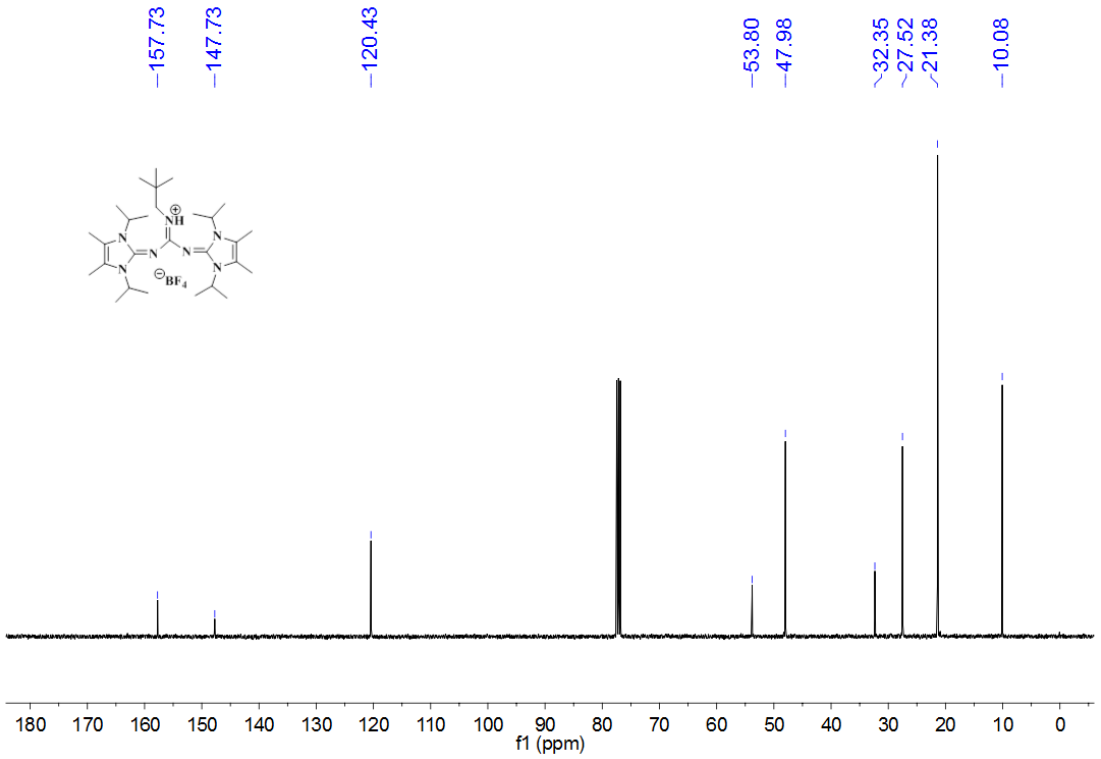
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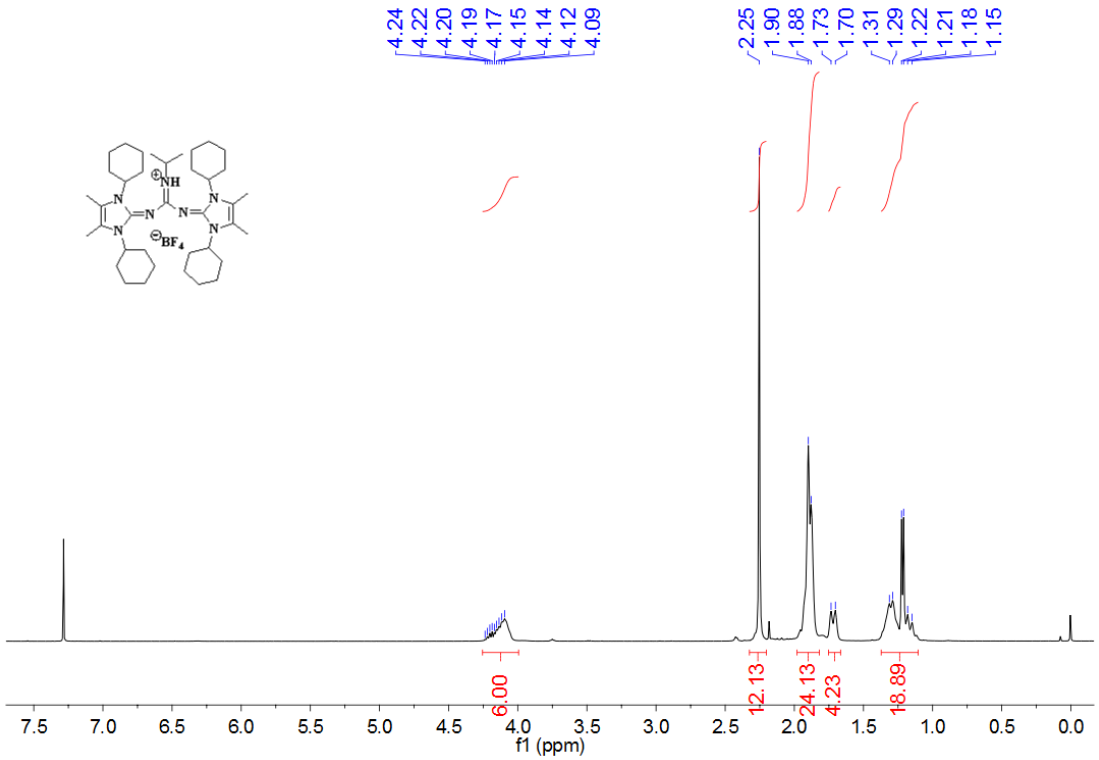
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1.73
1.70
1.31
1.29
1.22
1.21
1.18
1.15
6.00
12.13
24.13
4.23
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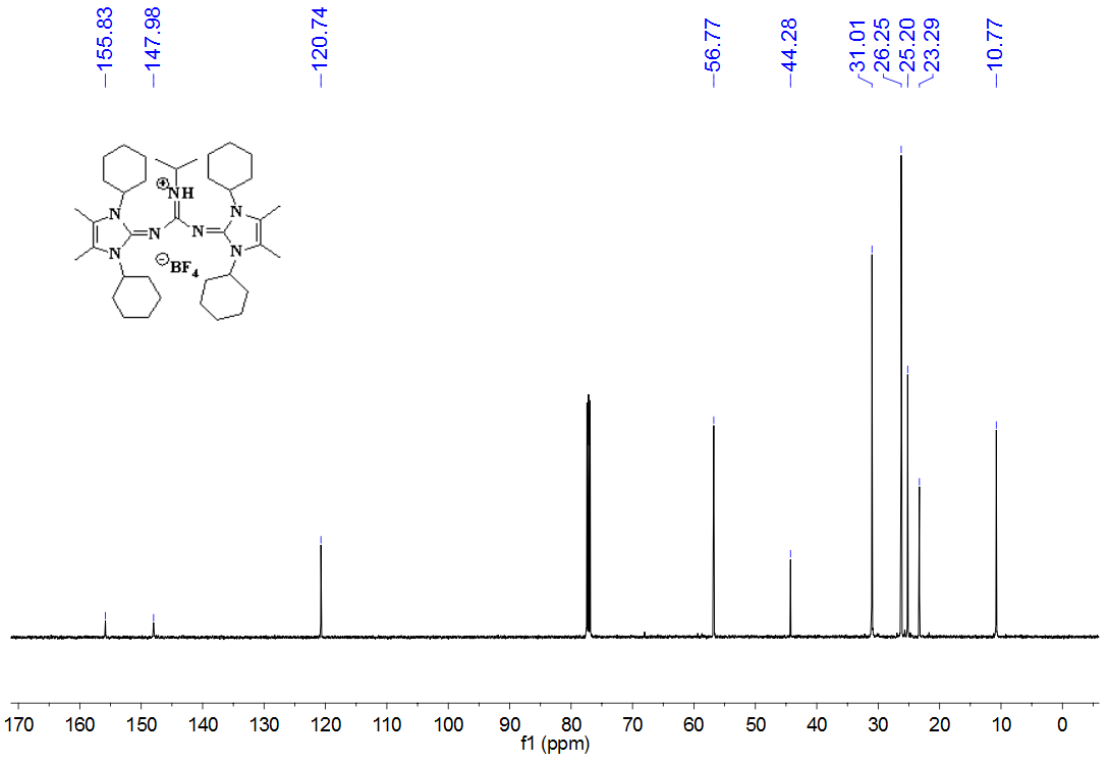
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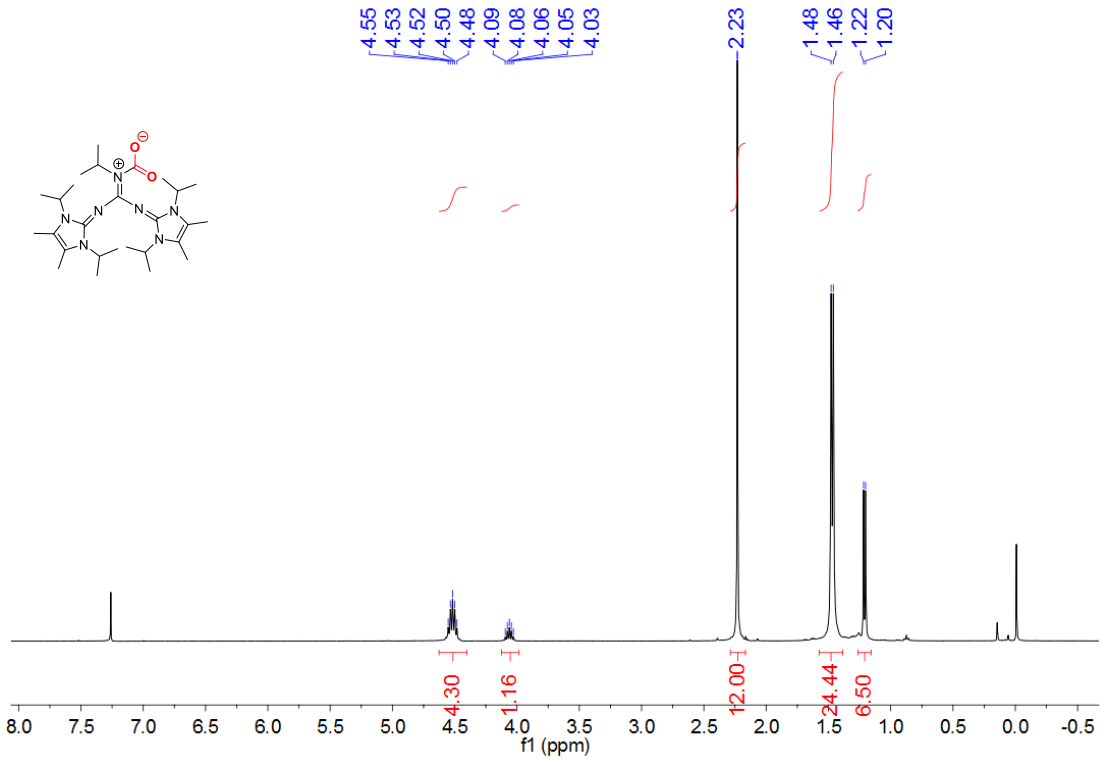
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1.22
1.20
4.30
1.16
12.00
24.44
6.50
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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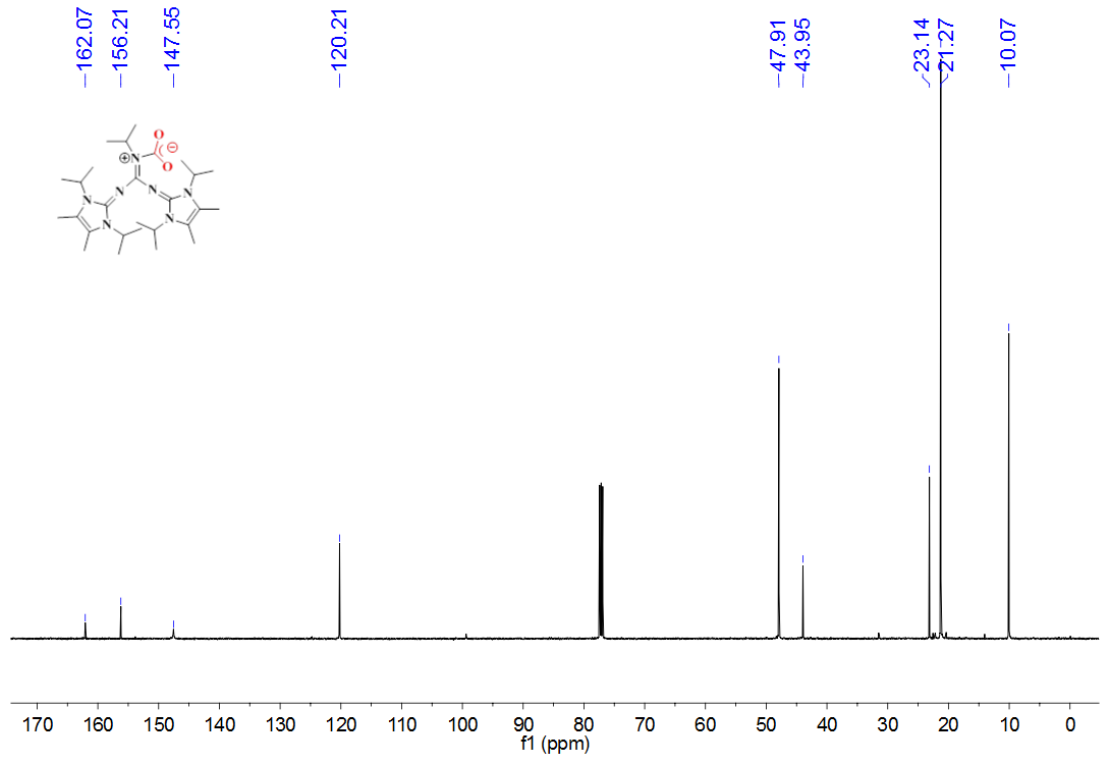
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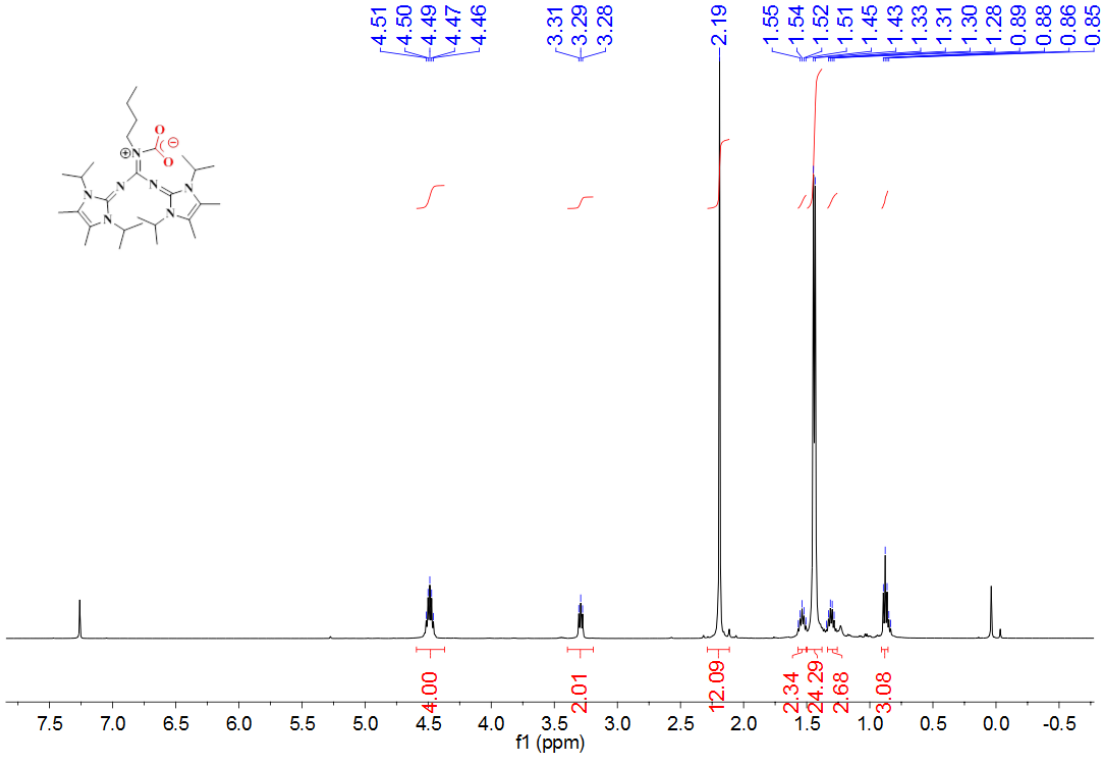
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1.45
1.43
1.33
1.31
1.30
1.28
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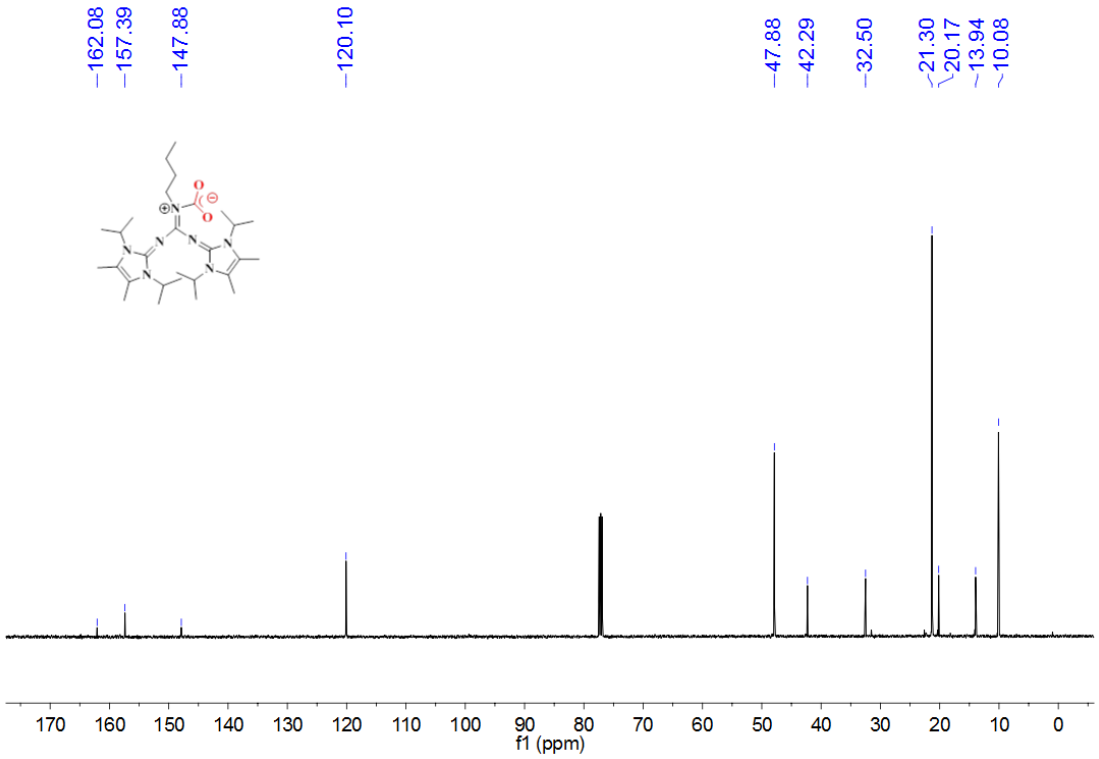
3.08
f1 (ppm)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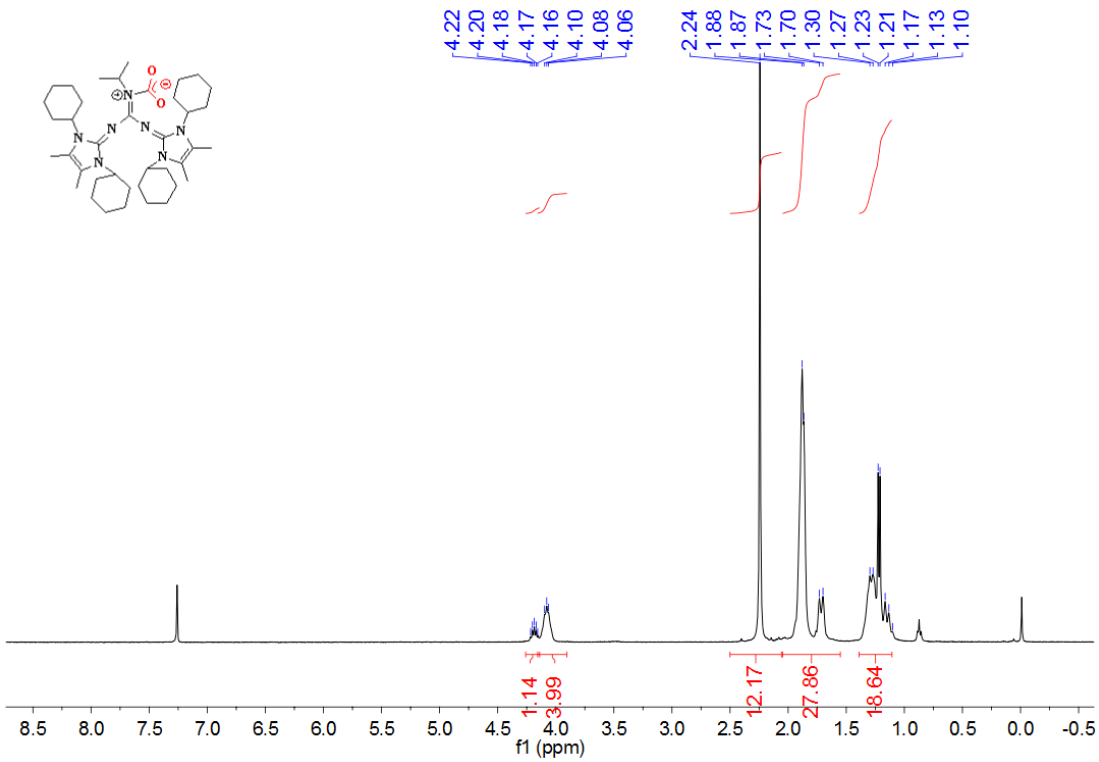
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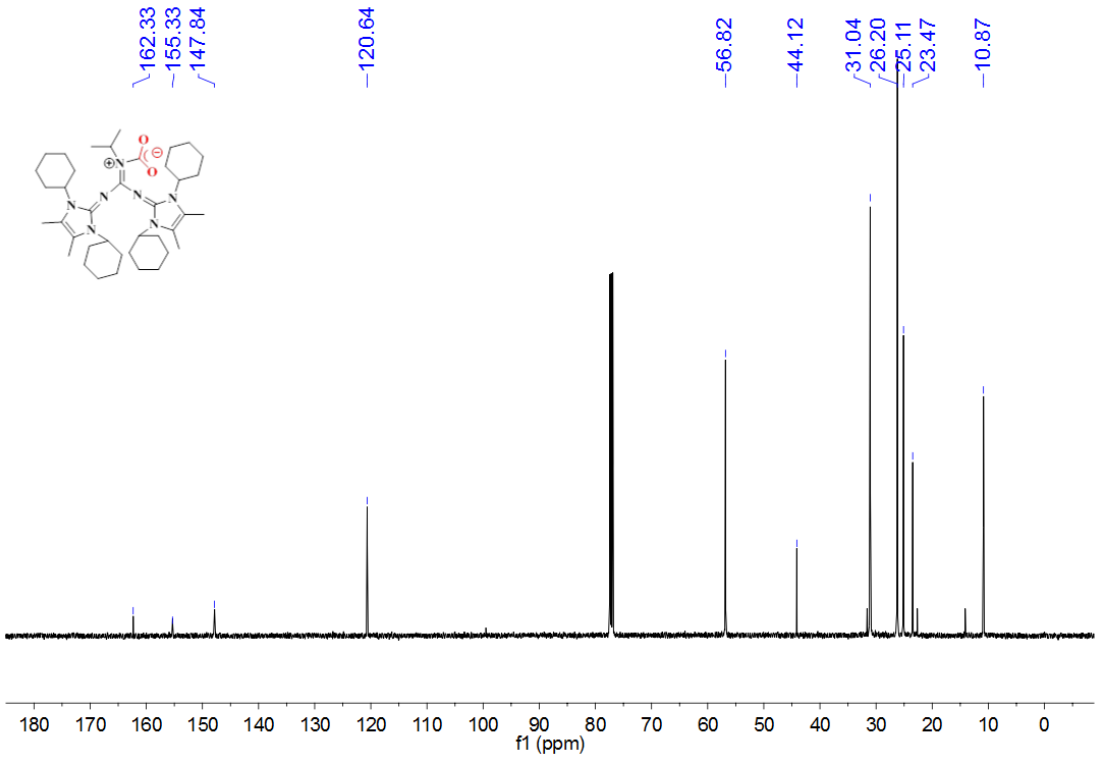
1.30
1.27
1.23
1.21
1.17
1.13
1.10
1.14
3.99
12.17
27.86
18.64
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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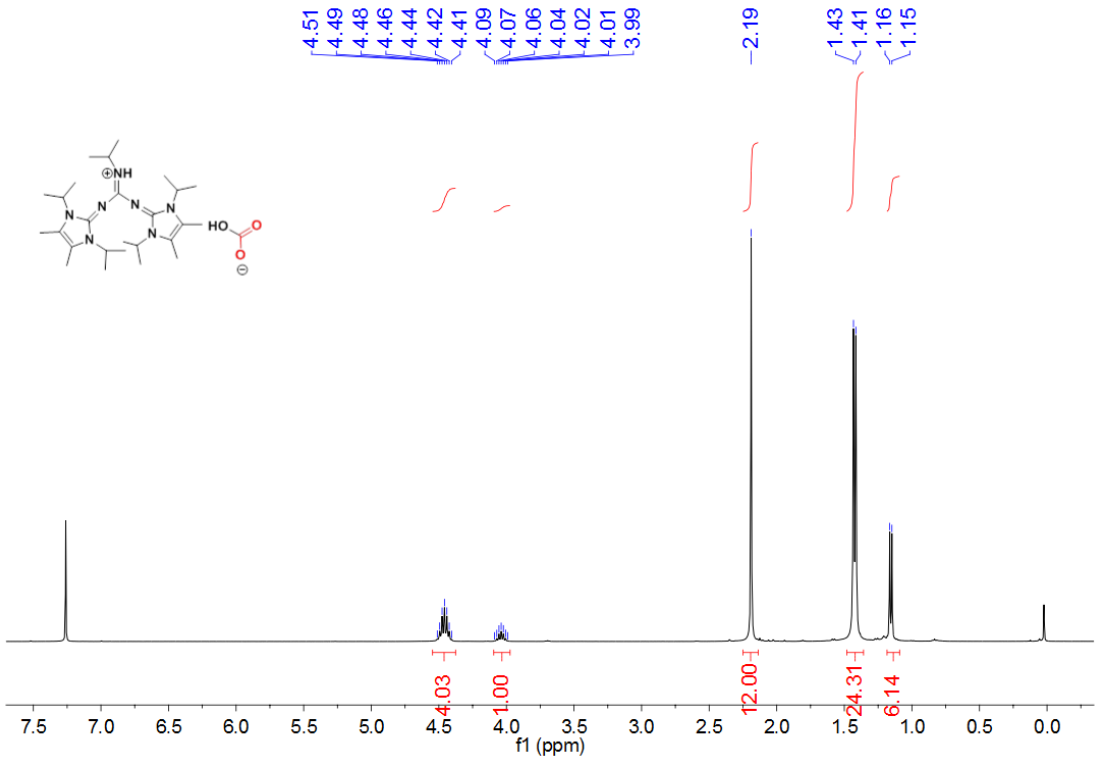
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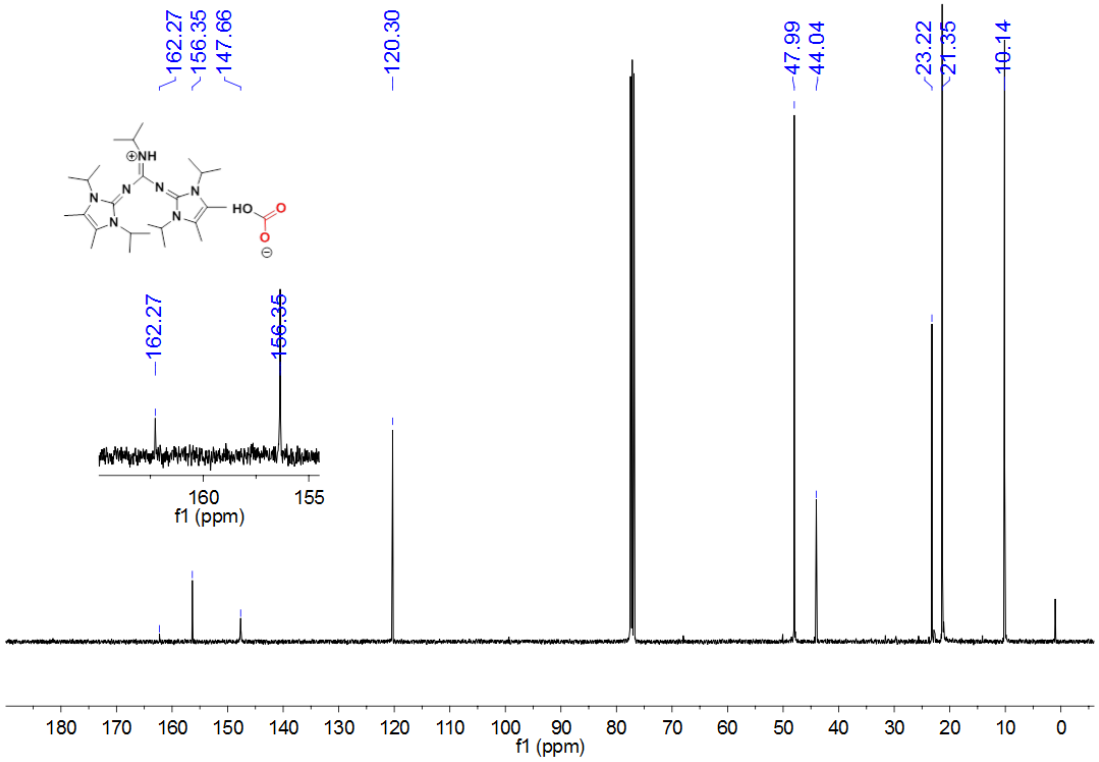
f1 (ppm)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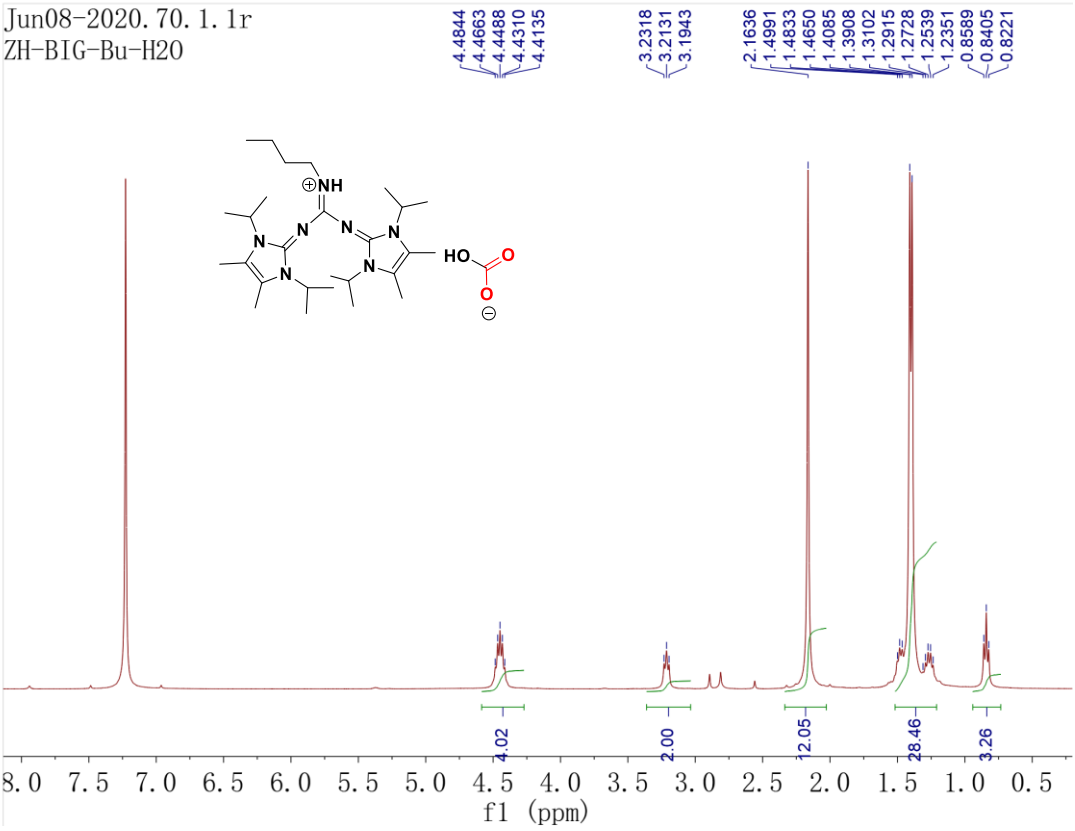
f1 (ppm)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NH
HO
O
O
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2.00
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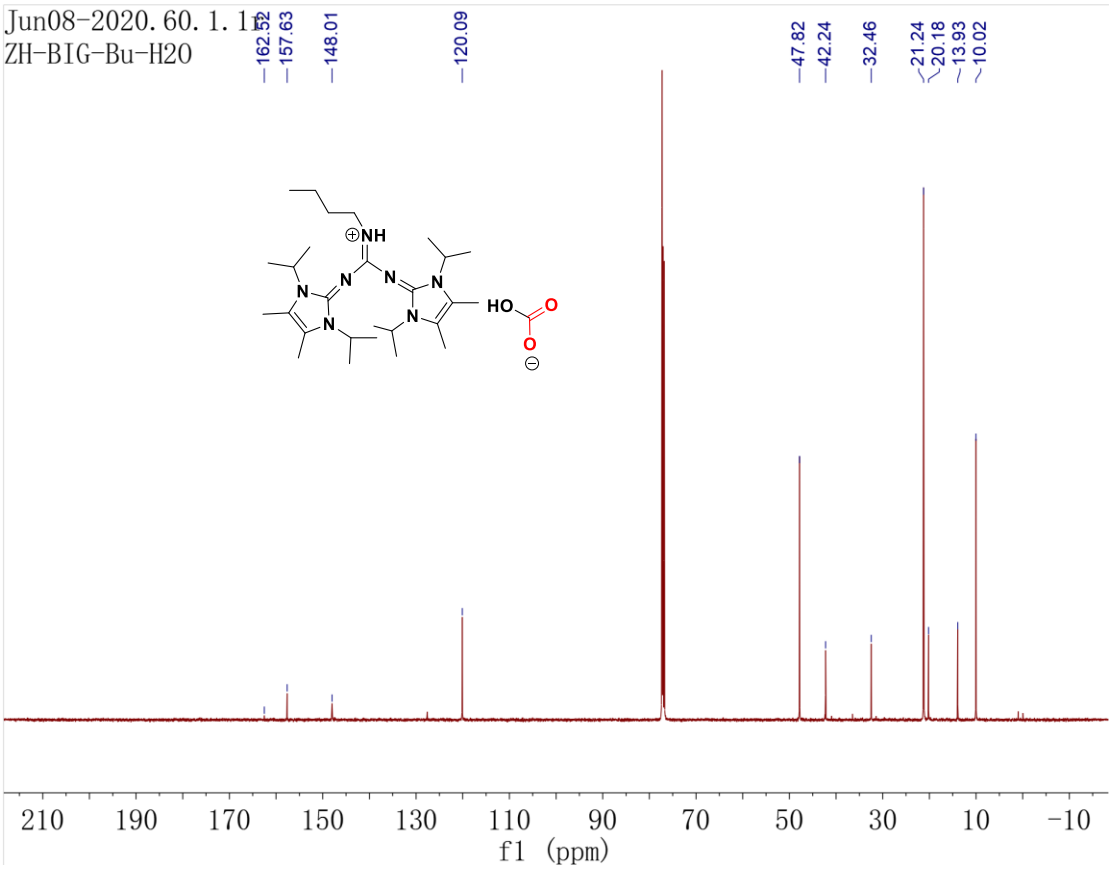
f1 (ppm)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O
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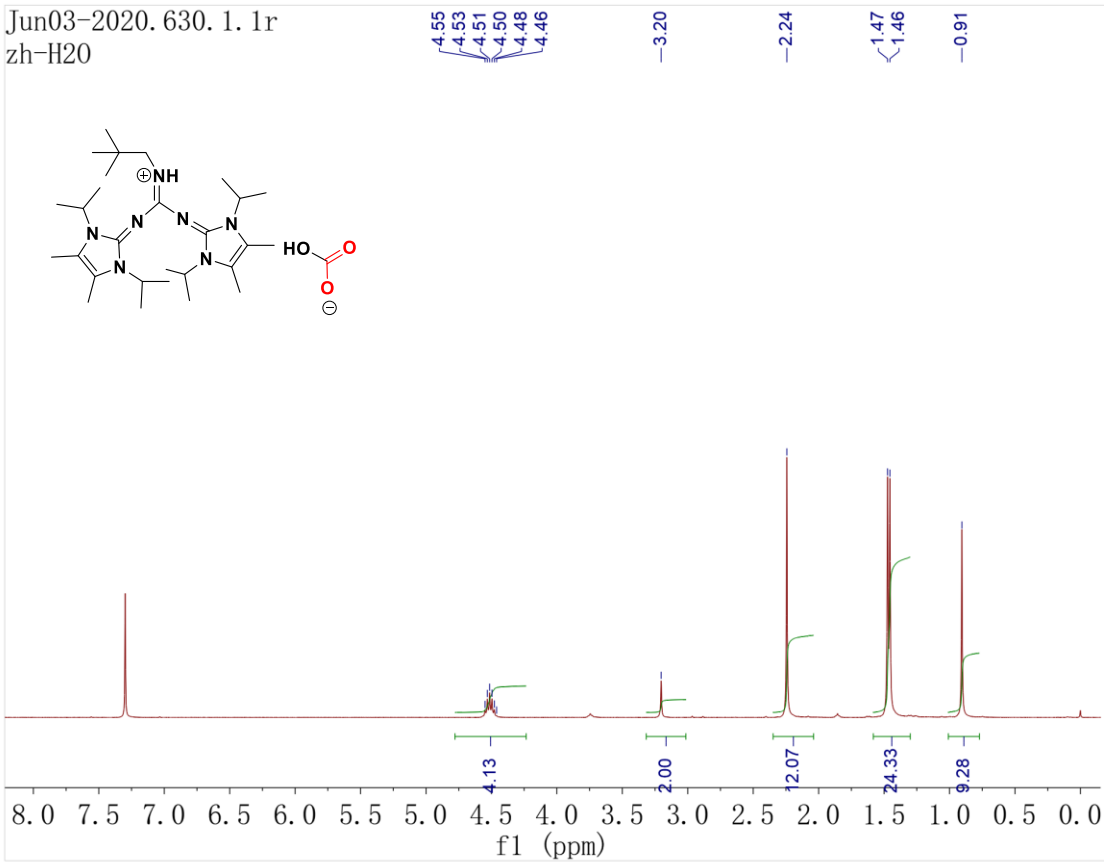
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24.33
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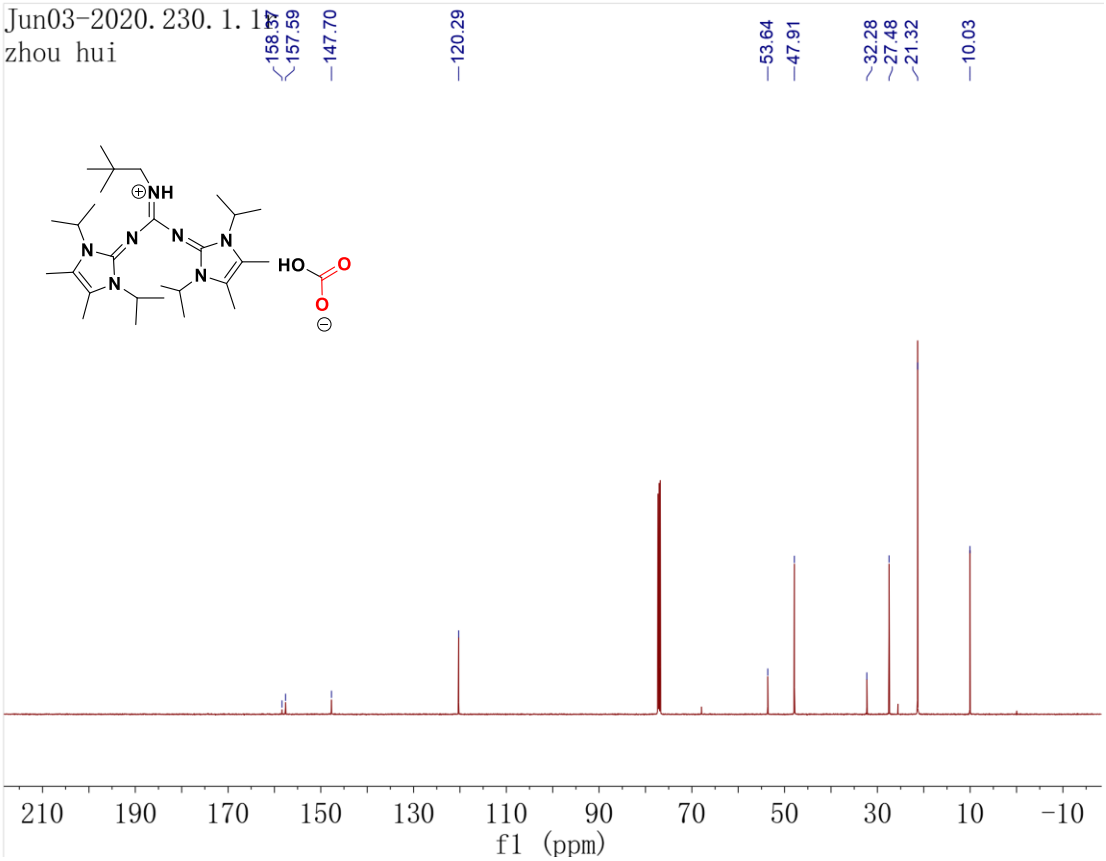
f1 (ppm)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32.28
27.48
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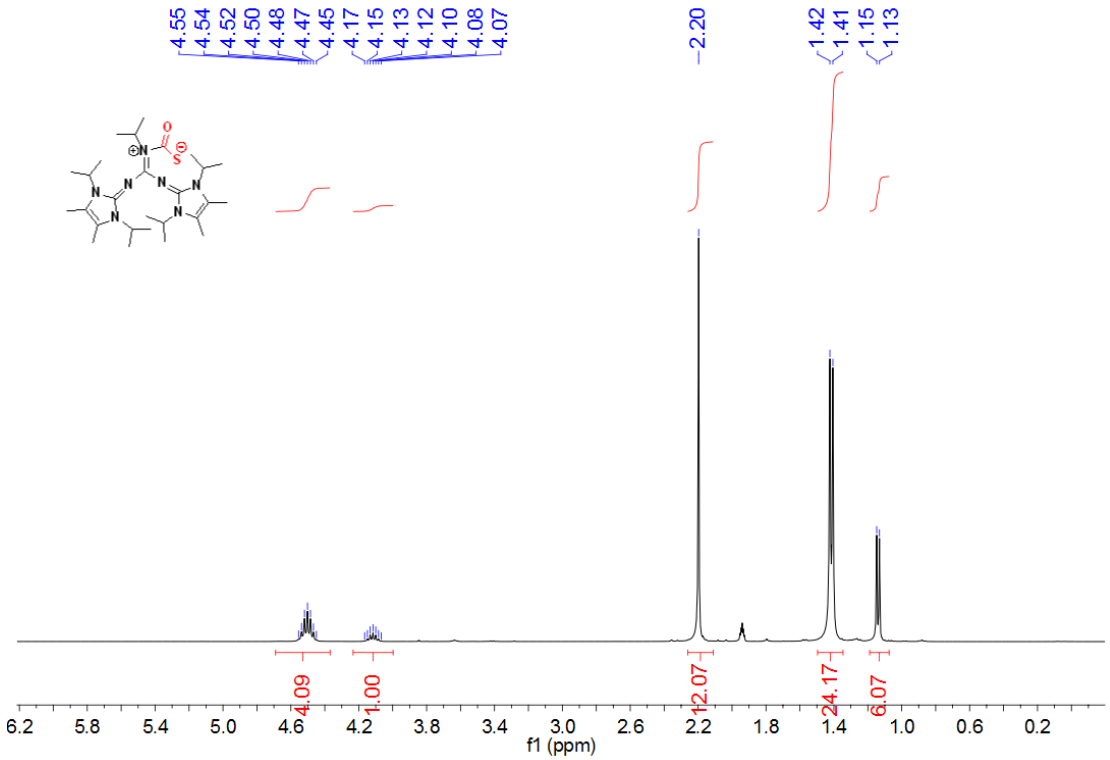
10.03
210 190 170 150 130 110 90 70 50 30 10 -10
f1 (ppm)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4.12
4.10
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1.42
1.41
1.15
1.13
4.09
1.00
12.07
24.17
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6.2
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4.2
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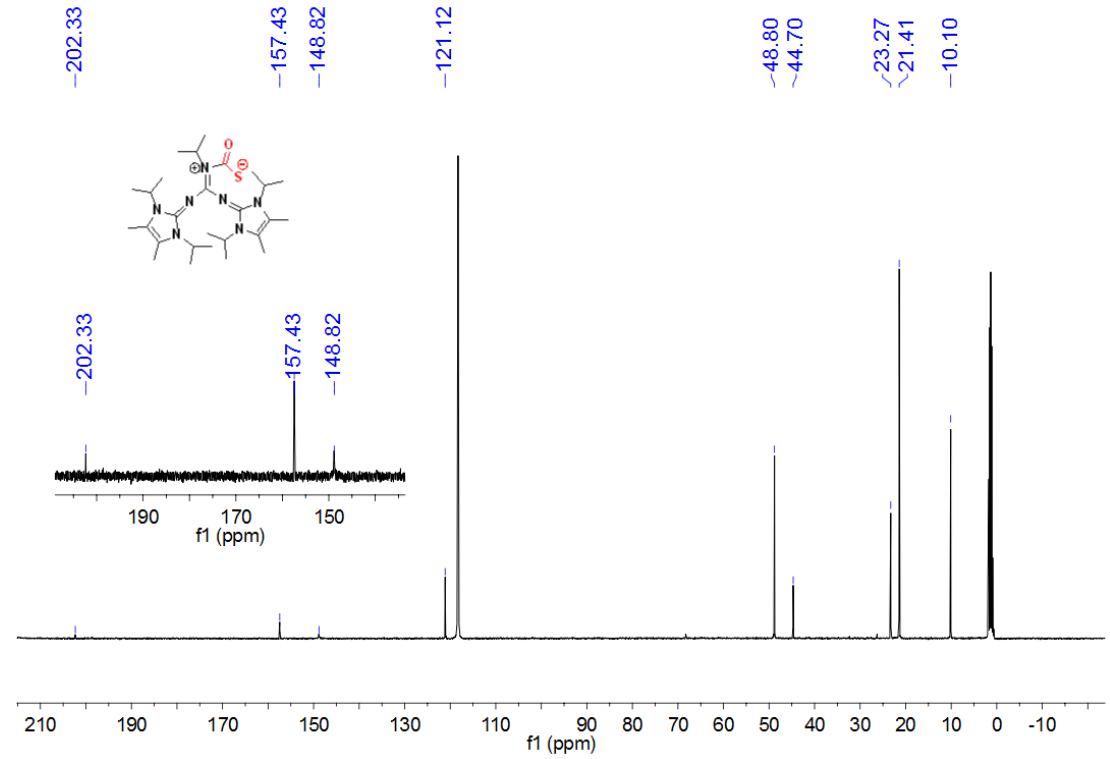
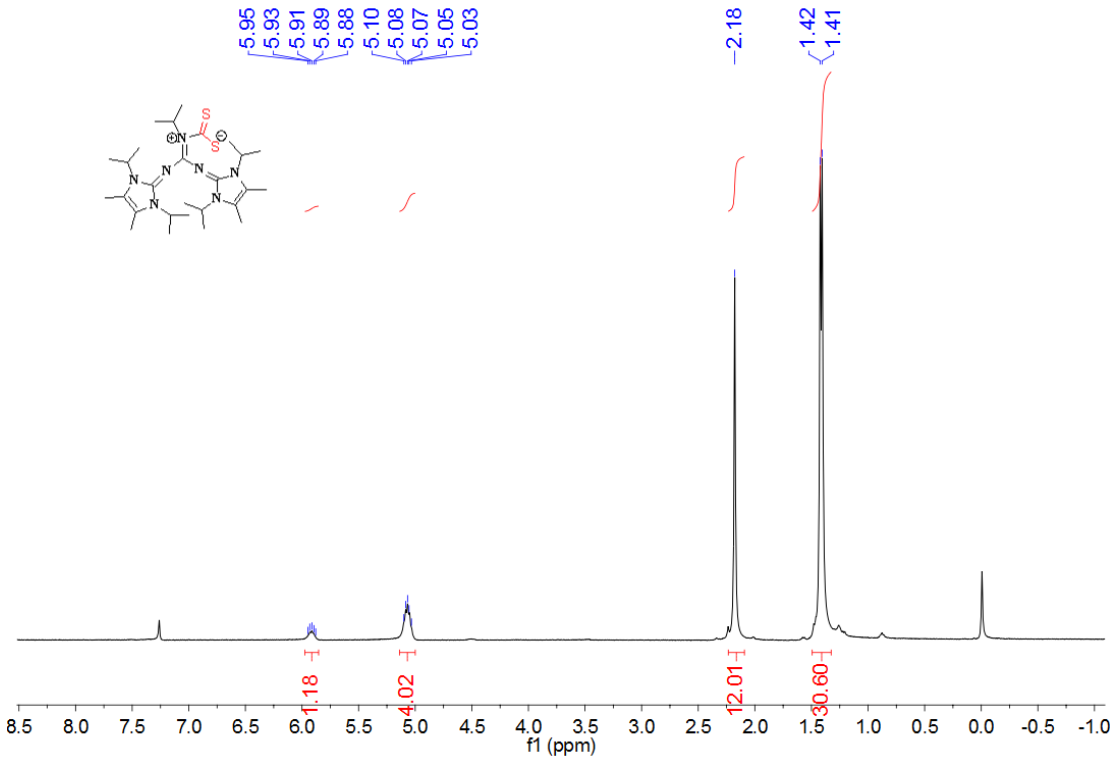
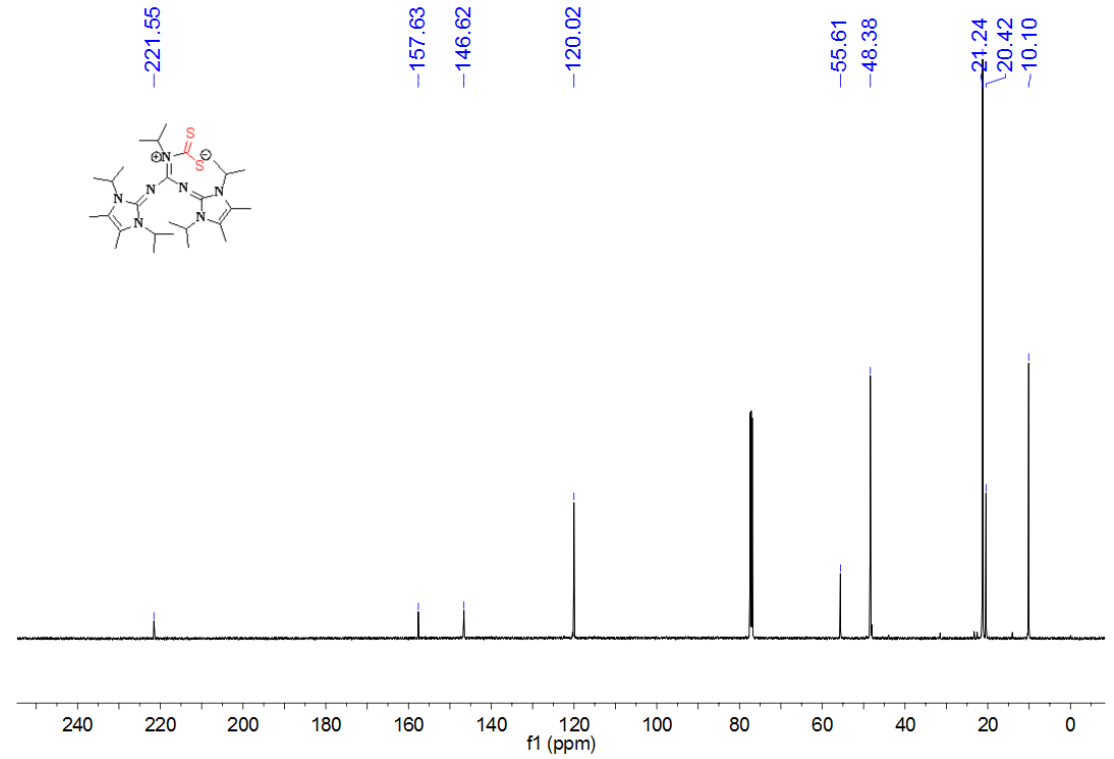
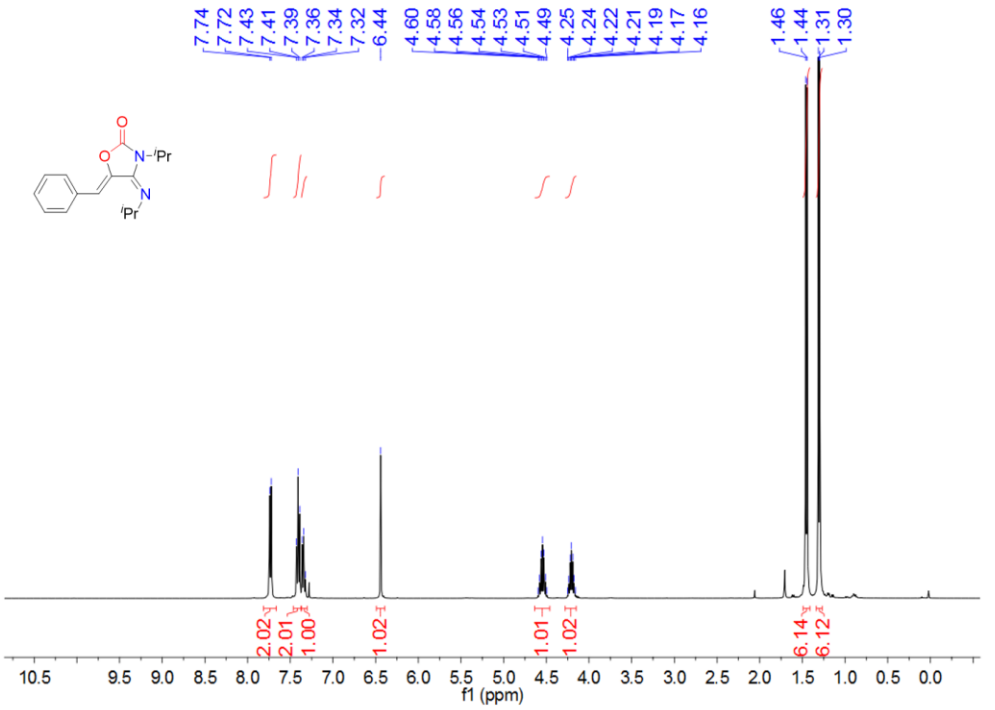
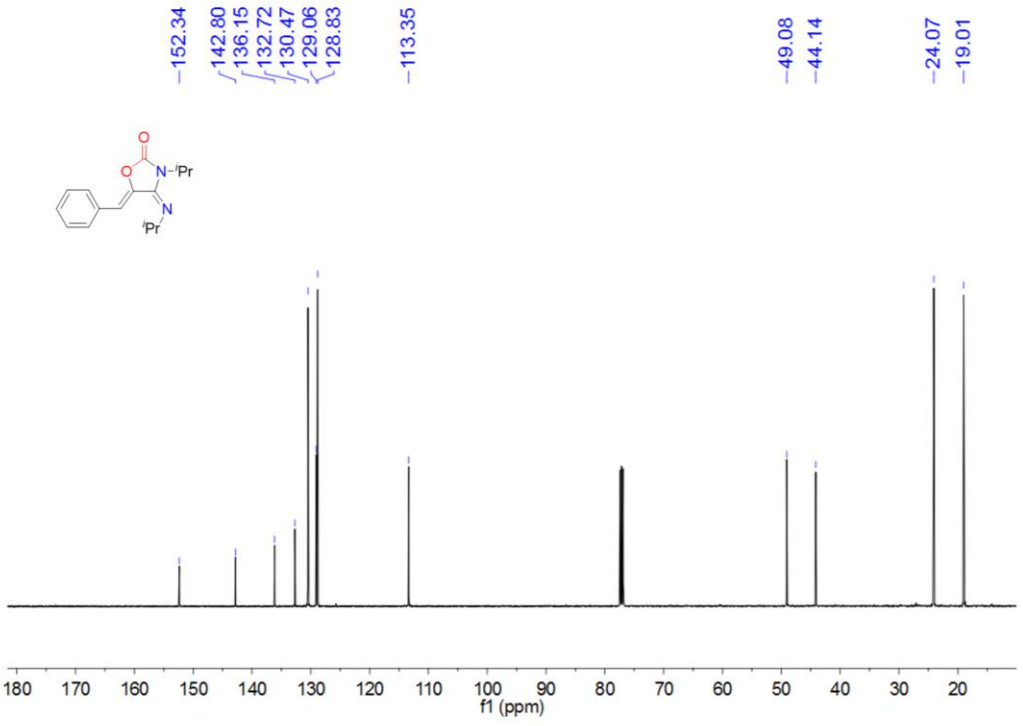
3.4
3.0
2.6
2.2
1.8
1.4
1.0
0.6
0.2
f1 (ppm)

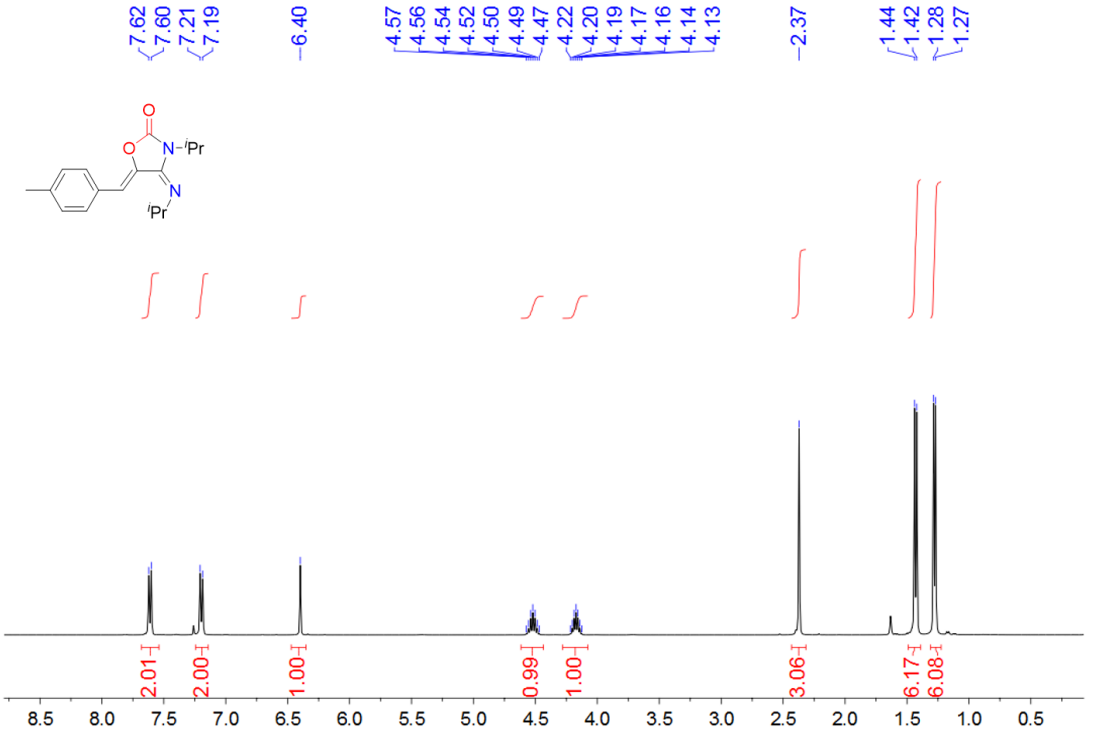

202.33
157.43
148.82
121.12
48.80
44.70
23.27
21.41
10.10
190
170
150
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

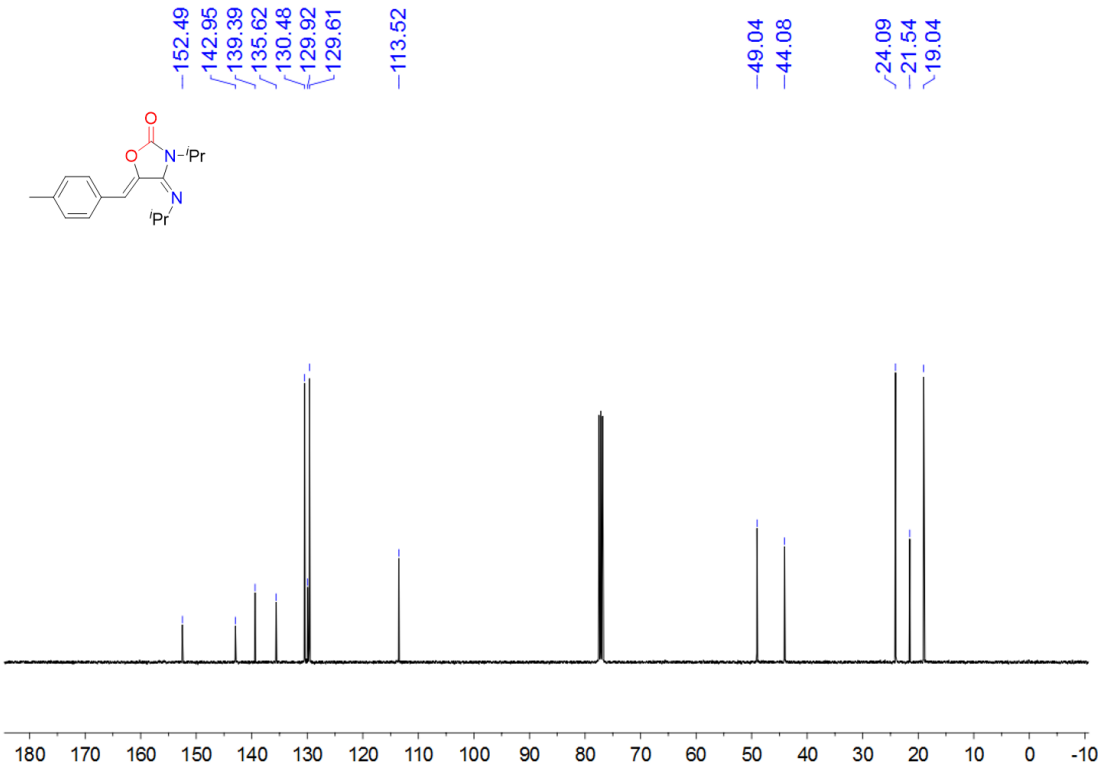

5.95
5.93
5.91
5.89
5.88
5.10
5.08
5.07
5.05
5.03
2.18
1.42
1.41
1.18
4.02
12.01
30.60
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

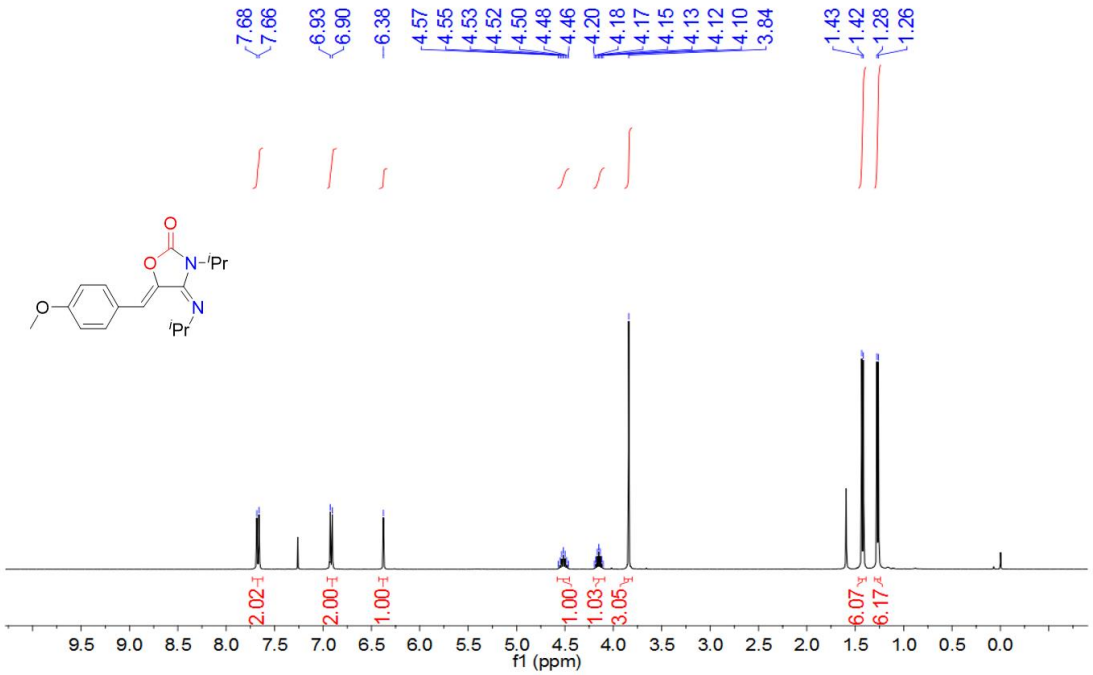

221.55
157.63
146.62
120.02
55.61
48.38
21.24
20.42
10.10
240 220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

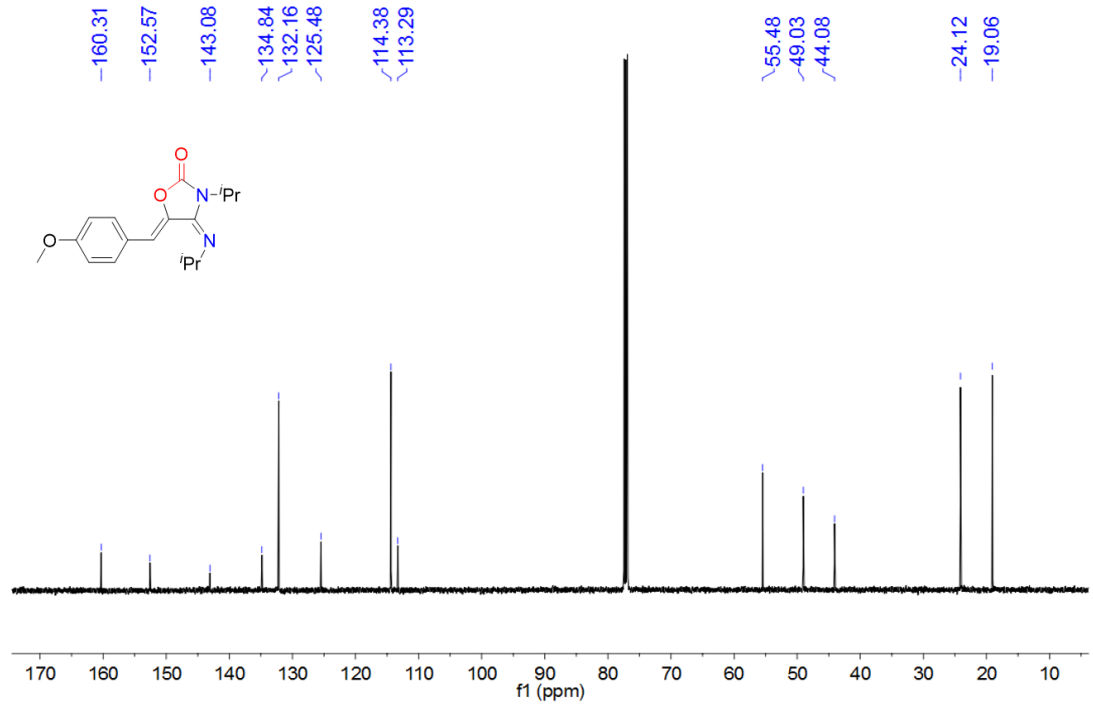

7.74
7.72
7.43
7.41
7.39
7.36
7.34
7.32
6.44
4.60
4.58
4.56
4.54
4.53
4.51
4.49
4.25
4.24
4.22
4.21
4.19
4.17
4.16
1.46
1.44
1.31
1.30
2.02
2.01
1.00
1.02
1.01
1.02
6.14
6.12
f1 (ppm)

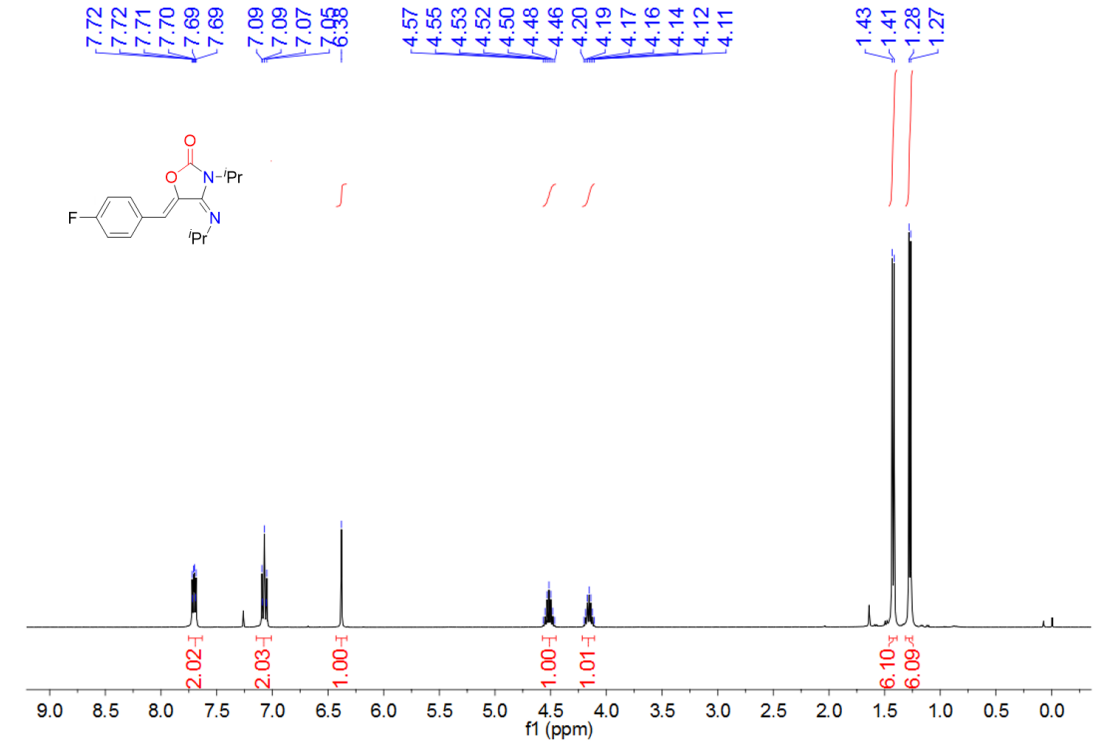

152.34
142.80
136.15
132.72
130.47
129.06
128.83
113.35
49.08
44.14
24.07
19.01
f1 (ppm)

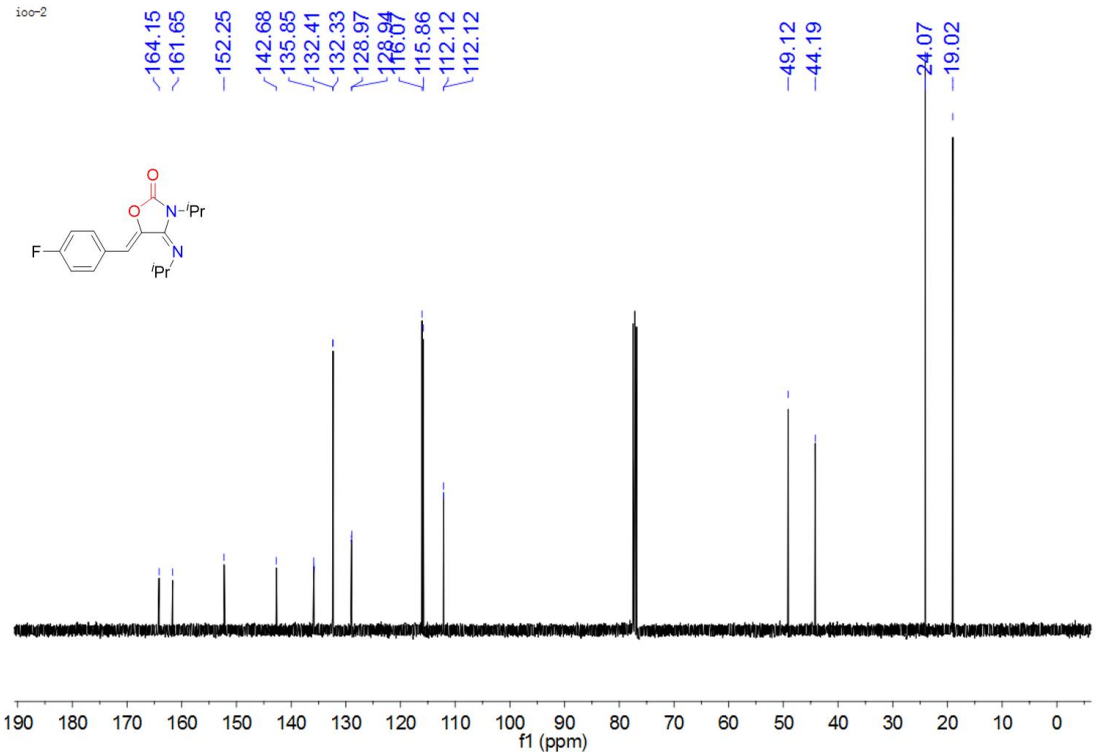

7.62
7.60
7.21
7.19
6.40
4.57
4.56
4.54
4.52
4.50
4.49
4.47
4.22
4.20
4.19
4.17
4.16
4.14
4.13
2.37
1.44
1.42
1.28
1.27
O
O
N-iPr
N
iPr
2.01
2.00
1.00
0.99
1.00
3.06
6.17
6.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5

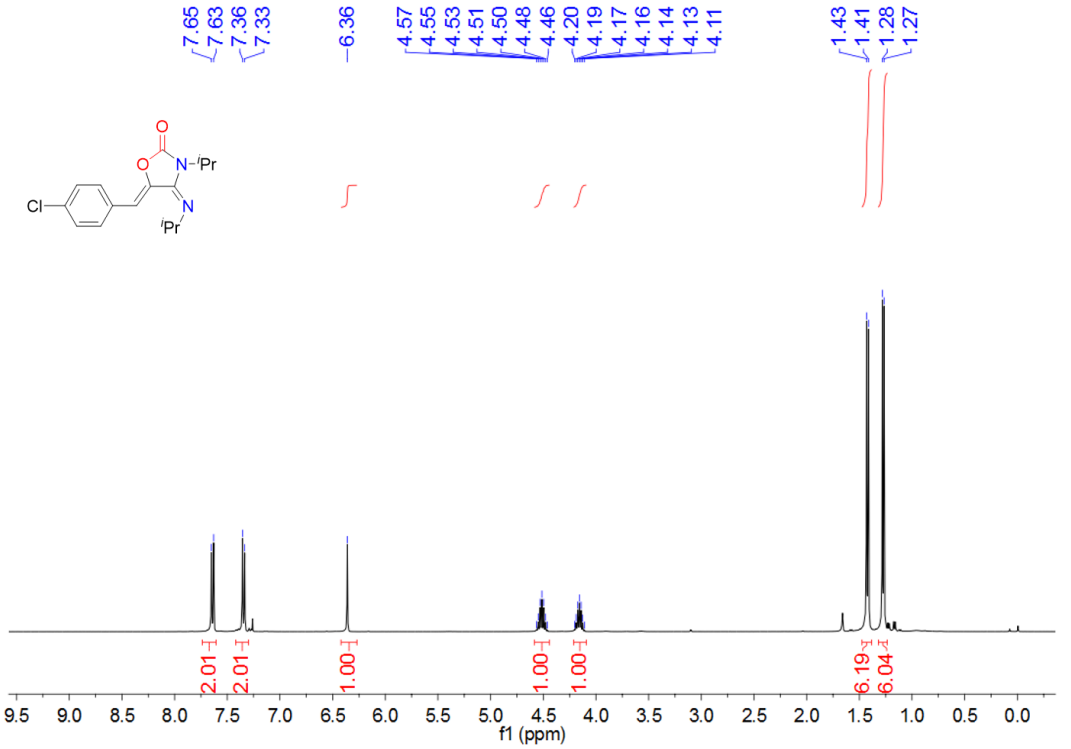

152.49
142.95
139.39
135.62
130.48
129.92
129.61
113.52
49.04
44.08
24.09
21.54
19.04
O
O
N-iPr
N
iPr
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

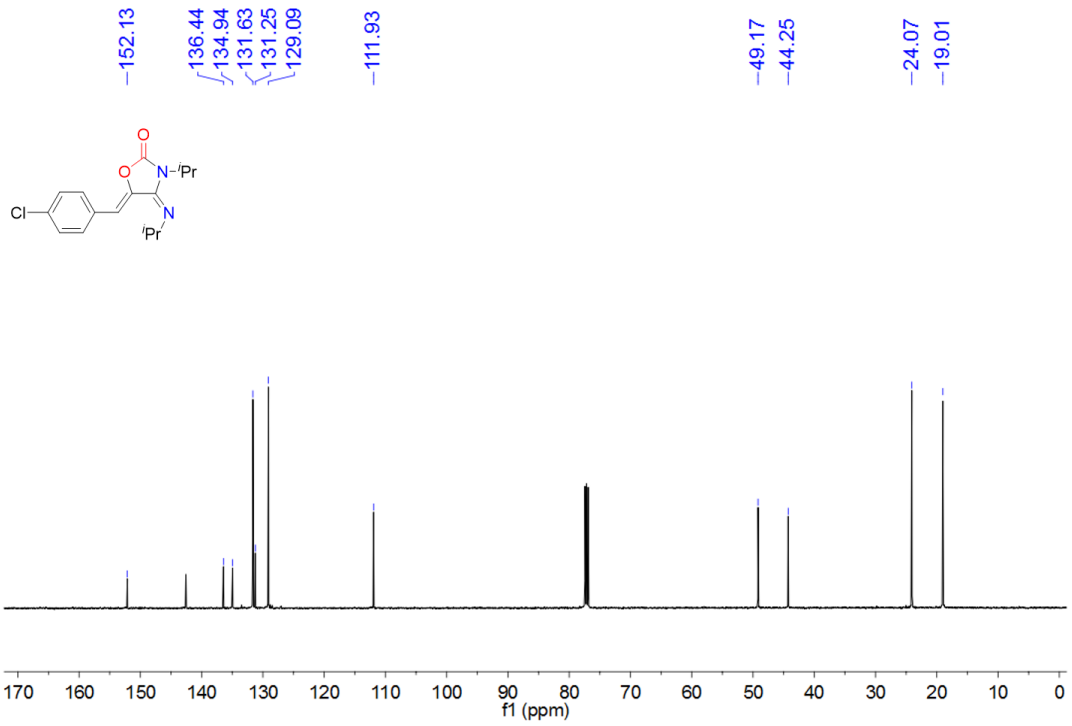

7.68
7.66
6.93
6.90
6.38
4.57
4.55
4.53
4.52
4.50
4.48
4.46
4.20
4.18
4.17
4.15
4.13
4.12
4.10
3.84
1.43
1.42
1.28
1.26
O
O
N-iPr
N
iPr
O
2.02
2.00
1.00
1.00
1.03
3.05
6.07
6.17
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

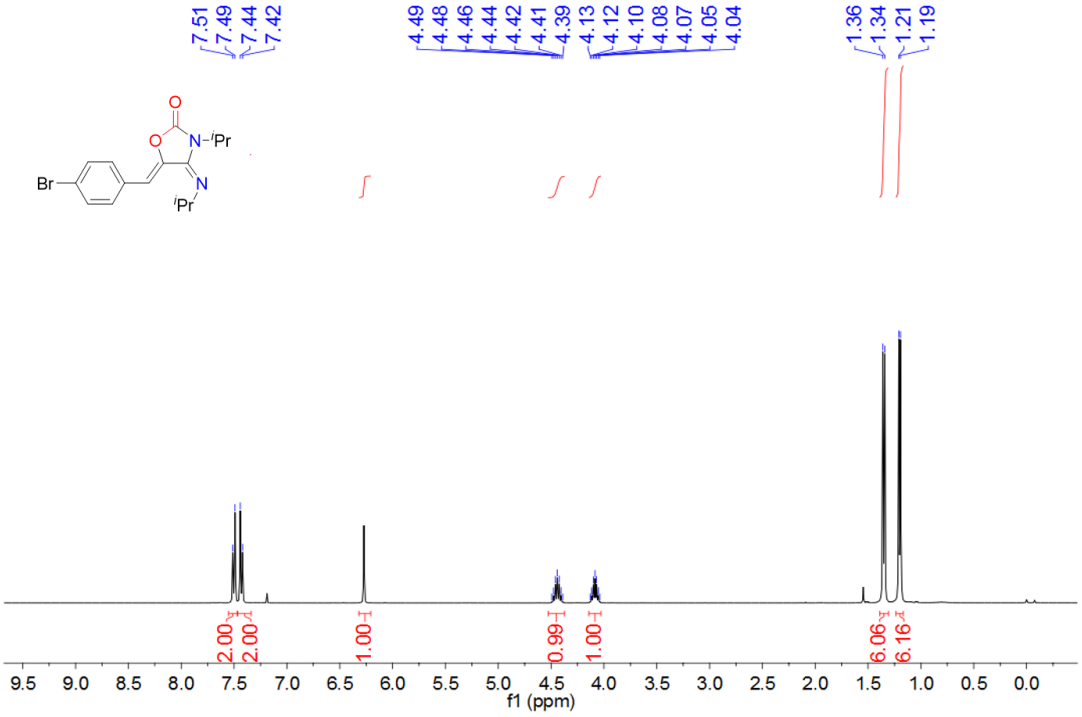

160.31
152.57
143.08
134.84
132.16
125.48
114.38
113.29
55.48
49.03
44.08
24.12
19.06
O
O
N-iPr
N
iPr
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

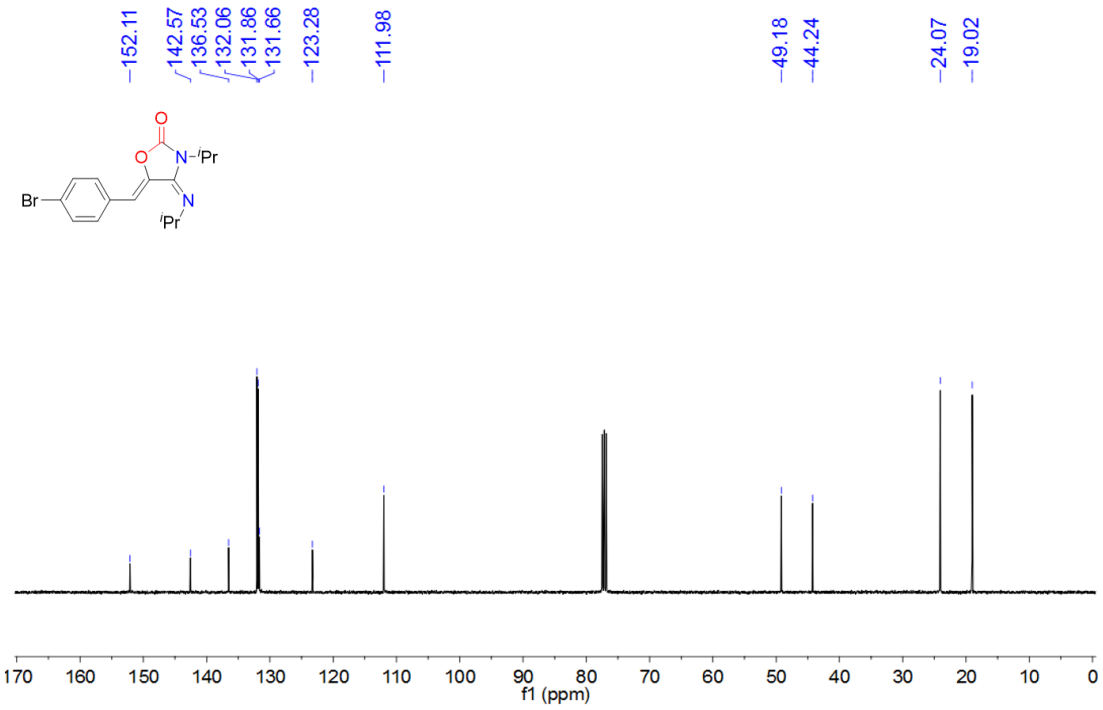

7.72
7.72
7.71
7.70
7.69
7.69
7.09
7.09
7.07
6.38
4.57
4.55
4.53
4.52
4.50
4.48
4.46
4.20
4.19
4.17
4.16
4.14
4.12
4.11
1.43
1.41
1.28
1.27
2.02
2.03
1.00
1.00
1.01
6.10
6.09
f1 (ppm)

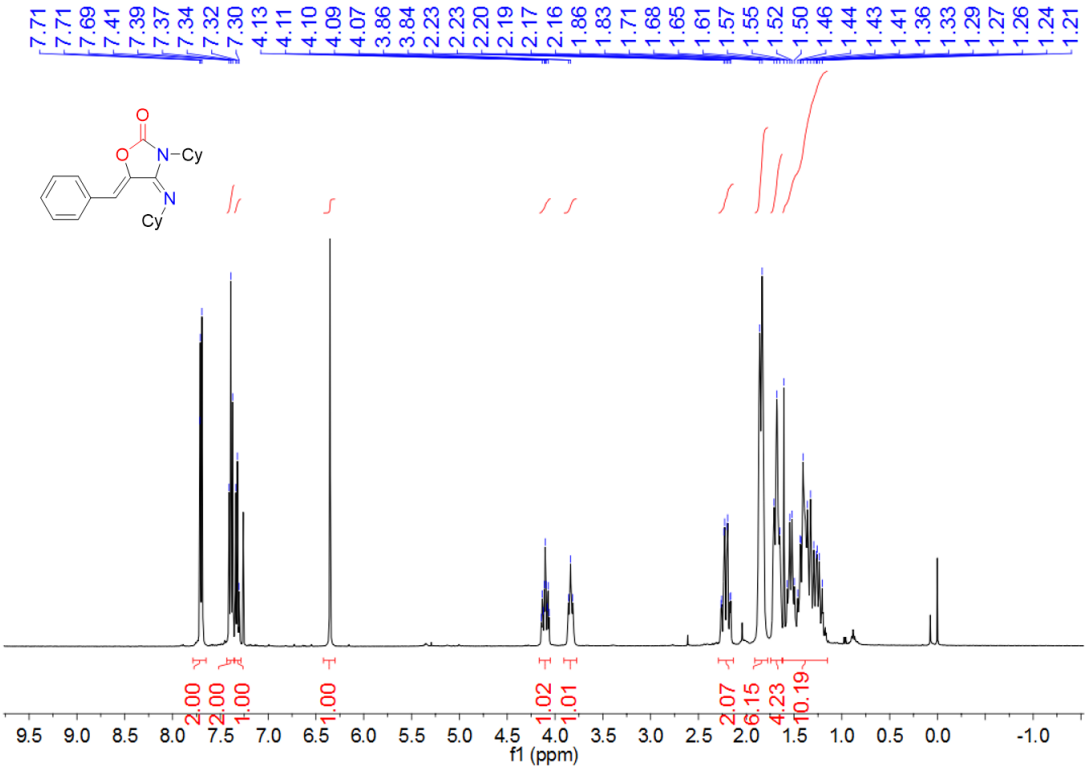

ioo-2
164.15
161.65
152.25
142.68
135.85
132.41
132.33
128.97
115.86
112.12
112.12
49.12
44.19
24.07
19.02
f1 (ppm)


7.65
7.63
7.36
7.33
6.36
4.57
4.55
4.53
4.51
4.50
4.48
4.46
4.20
4.19
4.17
4.16
4.14
4.13
4.11
1.43
1.41
1.28
1.27
Cl
O
O
N
iPr
N
iPr
2.01
2.01
1.00
1.00
1.00
6.19
6.04
9.5 9.0 8.5 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 1.0 0.5 0.0
f1 (ppm)


152.13
136.44
134.94
131.63
131.25
129.09
111.93
49.17
44.25
24.07
19.01
Cl
O
O
N
iPr
N
iPr
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.51
7.49
7.44
7.42
4.49
4.48
4.46
4.44
4.42
4.41
4.39
4.13
4.12
4.10
4.08
4.07
4.05
4.04
1.36
1.34
1.21
1.19
Br
O
N-iPr
N
iPr
2.00
2.00
1.00
0.99
1.00
6.06
6.16
9.5 9.0 8.5 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 1.0 0.5 0.0
f1 (ppm)


152.11
142.57
136.53
132.06
131.86
131.66
123.28
111.98
49.18
44.24
24.07
19.02
Br
O
N-iPr
N
iPr
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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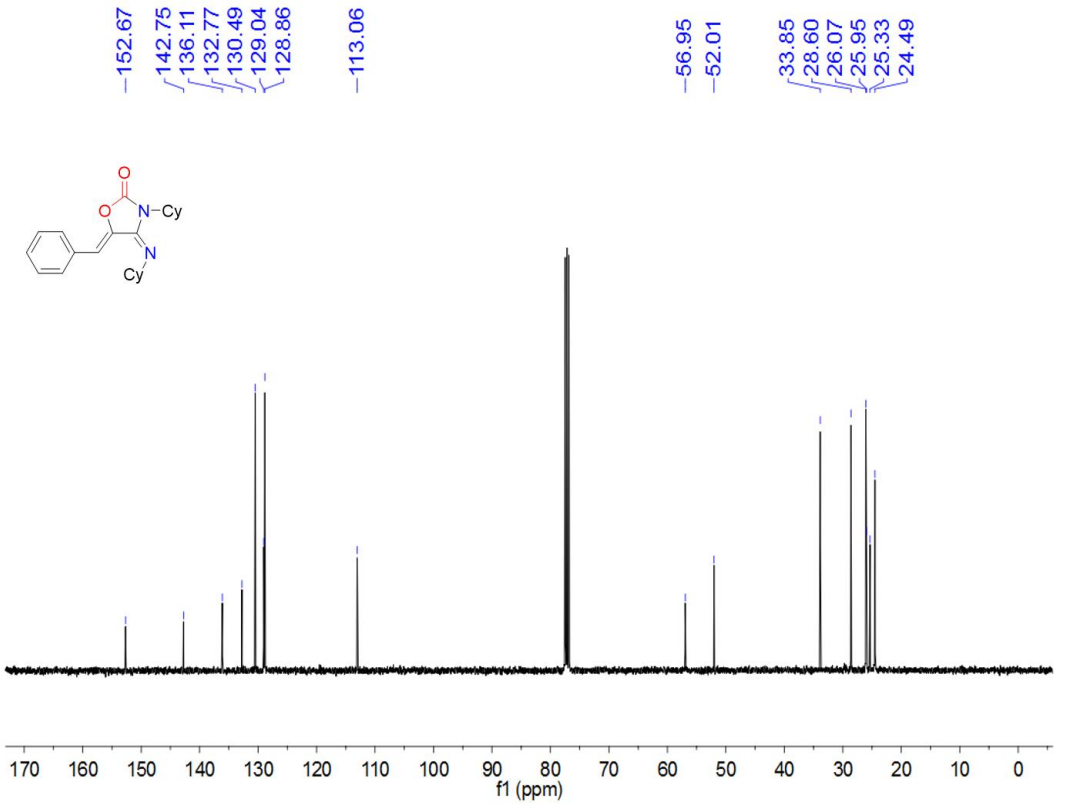
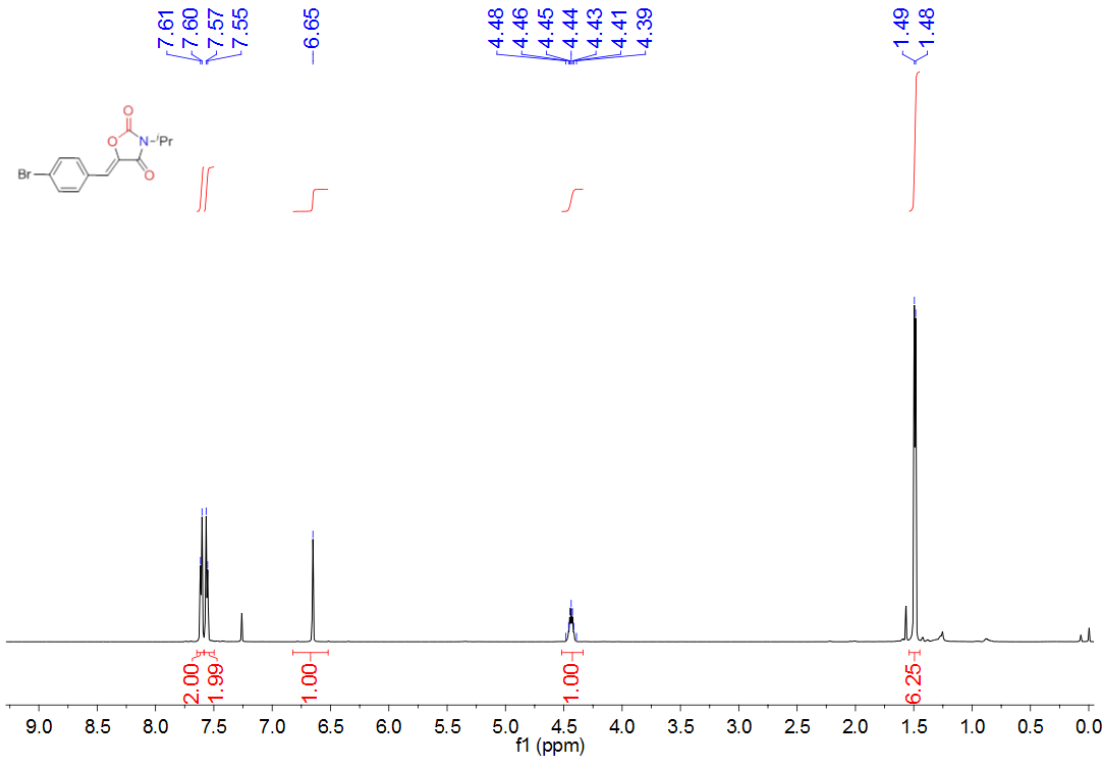
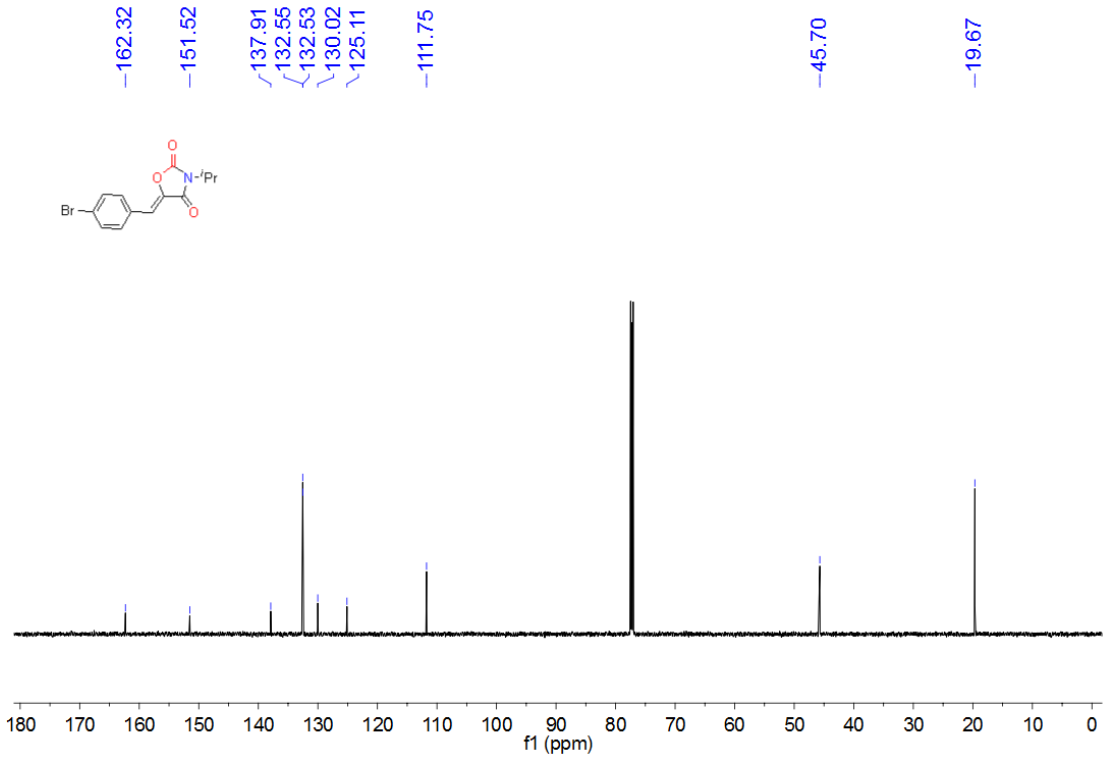
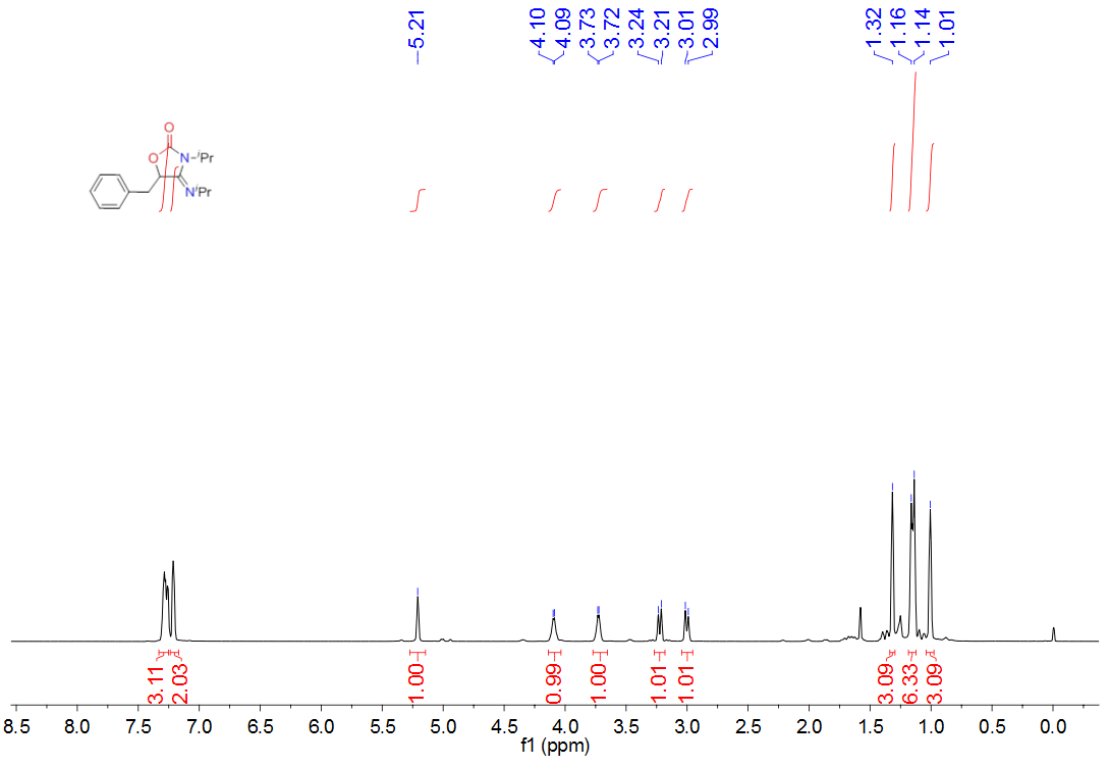
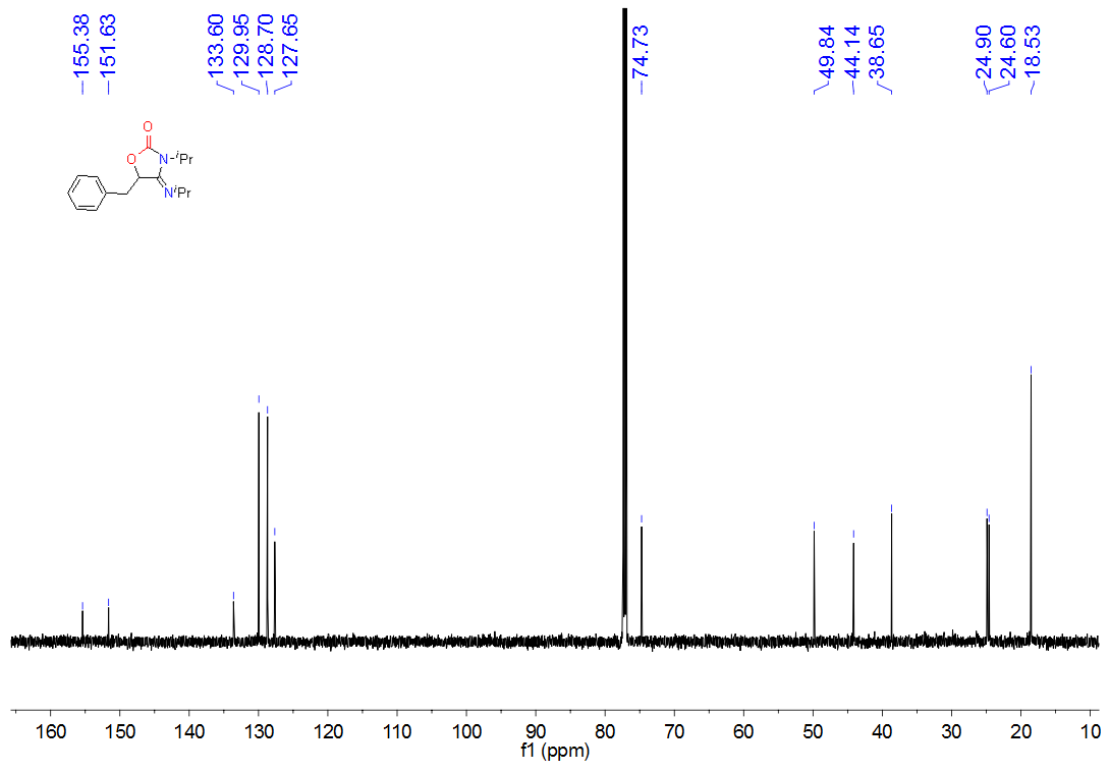
7.71
7.69
7.41
7.39
7.37
7.34
7.32
7.30
4.13
4.11
4.10
4.09
4.07
3.86
3.84
2.23
2.20
2.19
2.17
2.16
1.86
1.83
1.71
1.68
1.65
1.61
1.57
1.55
1.52
1.50
1.46
1.44
1.43
1.41
1.36
1.33
1.29
1.27
1.26
1.24
1.21
O
O
N–Cy
N
Cy
2.00
2.00
1.00
1.00
1.02
1.01
2.07
6.15
4.23
10.19
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)


152.67
142.75
136.11
132.77
130.49
129.04
128.86
113.06
56.95
52.01
33.85
28.60
26.07
25.95
25.33
24.49
O
O
N–Cy
N
Cy
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

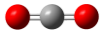

7.61
7.60
7.57
7.55
6.65
4.48
4.46
4.45
4.44
4.43
4.41
4.39
1.49
1.48
Br
N-iPr
2.00
1.99
1.00
1.00
6.25
f1 (ppm)


162.32
151.52
137.91
132.55
132.53
130.02
125.11
111.75
45.70
19.67
Br
N-iPr
f1 (ppm)

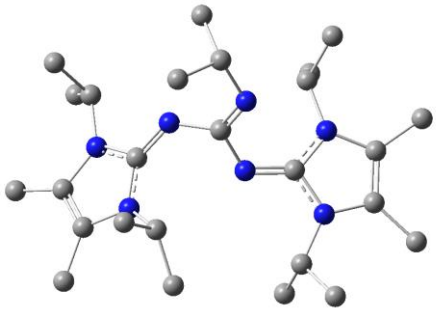

5.21
4.10
4.09
3.73
3.72
3.24
3.21
3.01
2.99
1.32
1.16
1.14
1.01
3.11
2.03
1.00
0.99
1.00
1.01
1.01
3.09
6.33
3.09
f1 (ppm)


155.38
151.63
133.60
129.95
128.70
127.65
74.73
49.84
44.14
38.65
24.90
24.60
18.53
f1 (ppm)

12. **Cartesian coordinates of BIG, BIG-CO_2 and TS**



O	0. 00000	0.00000	1.15606
O	0. 00000	0. 00000	-1.15606
C	0. 00000	0. 00000	0.00000



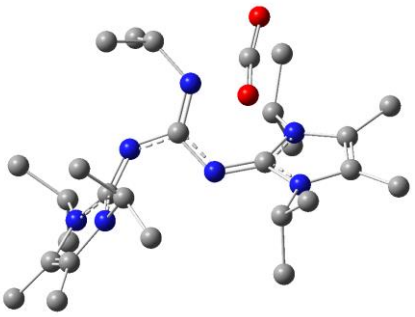
2a

N	-0.75103	0.22587	0.07750
N	-2.83053	1.28318	-0.22261
N	3.06322	-0.41487	-0.91094
N	2.2388	1.28147	0.22028
N	-2.86255	-0.90383	-0.3944
N	1.24609	-0.93337	0.47052
N	-0.68539	-1.39335	1.75068
C	-2.03656	0.16252	-0.12588
C	-0.07474	-0.73508	0.82561
C	2.05551	-0.05907	-0.04053
C	1.5765	1.94371	1.34716
H	0.68257	1.34212	1.53924
C	-2.25964	2.61098	-0.03212
H	-1.33056	2.39708	0.51075
C	3.39698	1.72628	-0.43648
C	3.90897	0.67455	-1.12731
C	0.01861	-2.35482	2.58237
H	-0.73204	-2.71436	3.30878
C	-2.35151	-2.24638	-0.68784

H	-1.28322	-2.19504	-0.46018
C	-4.13091	0.91822	-0.57479
C	-2.47197	-2.5783	-2.17516
H	-3.51263	-2.69737	-2.50567
H	-1.94787	-3.52264	-2.38074
H	-2.00515	-1.78784	-2.77953
C	3.2237	-1.80905	-1.31636
H	2.22828	-2.23563	-1.13298
C	3.87879	3.13867	-0.41185
H	3.16652	3.82071	-0.89946
H	4.83142	3.21091	-0.94948
H	4.0462	3.50625	0.61062
C	-4.15768	-0.43789	-0.65862
C	1.09034	3.35002	1.00083
H	1.89855	4.09295	1.01368
H	0.34299	3.66655	1.74304
H	0.61805	3.35321	0.00855
C	2.4587	1.90811	2.59332
H	2.71617	0.87041	2.84634
H	1.92185	2.34587	3.44725
H	3.39034	2.47509	2.44735
C	-3.11279	3.52917	0.83857
H	-3.96589	3.95743	0.29575
H	-2.49118	4.36823	1.18312
H	-3.48616	2.99464	1.72331
C	3.54771	-1.97911	-2.79809
H	2.90118	-1.34086	-3.4167
H	3.36848	-3.02517	-3.08346
H	4.5966	-1.75264	-3.03081
C	-2.95187	-3.29579	0.23965

H	-2.78514	-2.97777	1.27804
H	-4.02595	-3.44447	0.06146
C	-1.87786	3.2389	-1.37007
H	-1.17439	2.58067	-1.89932
H	-1.39683	4.21592	-1.21324
H	-2.76328	3.39384	-2.00577
C	-5.34905	-1.32064	-0.83829
H	-6.21012	-0.71739	-1.1498
H	-5.19813	-2.09977	-1.59613
H	-5.6173	-1.82188	0.10422
C	-5.25054	1.88989	-0.74753
H	-5.58294	2.32148	0.20834
H	-4.96332	2.72102	-1.40774
H	-6.11005	1.38652	-1.20555
C	5.10398	0.63401	-2.0204
H	5.76757	-0.20611	-1.76987
H	4.82707	0.53689	-3.08063
H	5.68314	1.55778	-1.90751
C	4.2109	-2.52863	-0.40074
H	4.26433	-3.59637	-0.65799
H	5.22223	-2.10289	-0.49052
H	3.88217	-2.43898	0.6442
H	-2.45154	-4.26182	0.07957
C	1.155	-1.74305	3.41021
H	1.50187	-2.45229	4.17775
H	2.00496	-1.48075	2.7651
H	0.80245	-0.83138	3.91627
C	0.49867	-3.59075	1.81083
H	-0.33915	-4.04492	1.26084
H	1.28103	-3.31408	1.09132

H	0.90124	-4.34781	2.50187



TS 2a-3a

N	-0.47907	0.23563	-0.32291
O	-2.17292	0.75412	2.16817
O	-3.00706	-1.33089	2.70242
N	-2.4901	1.4003	-0.71451
N	3.37467	-0.44737	-0.84675
N	2.47614	1.22378	0.26075
N	-2.61984	-0.77833	-0.90182
N	1.41364	-0.9652	0.33003
N	-0.66388	-1.38123	1.34711
C	-1.76063	0.24797	-0.59906
C	0.07227	-0.72685	0.49542
C	2.29428	-0.09681	-0.07424
C	1.70163	1.86378	1.33033
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C	-2.15765	-2.13858	-1.20533
H	-1.10484	-2.14716	-0.91039
C	-3.79821	1.09976	-1.09134
C	-2.20528	-2.41059	-2.70847

H	-3.23045	-2.43901	-3.10227
H	-1.73971	-3.38413	-2.91836
H	-1.6464	-1.63683	-3.25341
C	3.54034	-1.82761	-1.2992
H	2.52265	-2.23467	-1.22986
C	4.21555	3.05985	-0.11656
H	3.57668	3.78366	-0.64342
H	5.221	3.1255	-0.54827
H	4.28401	3.37627	0.93395
C	-3.8852	-0.25315	-1.1958
C	1.30436	3.29978	0.99423
H	2.12481	4.013	1.1471
H	0.47702	3.60412	1.65151
H	0.96212	3.36616	-0.04788
C	2.42973	1.74695	2.66732
H	2.62986	0.6923	2.90091
H	1.80595	2.16376	3.47093
H	3.38576	2.29174	2.65655
C	-2.79247	3.54247	0.53754
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H	3.42771	-1.25651	-3.39546
H	3.82368	-2.96596	-3.10055
H	5.06964	-1.73055	-2.87283
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H	-2.8076	-2.90851	0.70073
H	-3.92094	-3.31258	-0.64848
C	-1.41094	3.42476	-1.60082

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H	-5.41604	-1.59982	-0.51796
C	-4.8652	2.12319	-1.29737
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H	-4.4956	2.9685	-1.89491
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H	6.15449	-0.27925	-1.42047
H	5.37374	0.54456	-2.78691
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H	3.99825	-2.55909	0.68373
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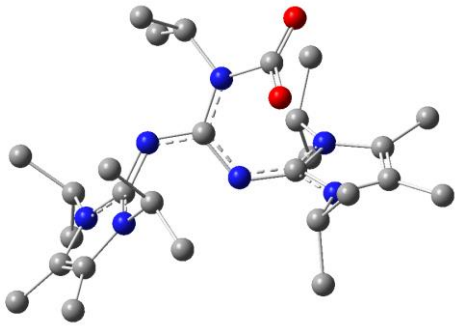

3a

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N	-0.71558	-1.27	1.43761
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C	-1.88543	2.68716	-0.24607
H	-0.95495	2.37213	0.23758
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C	-2.16448	-2.44462	-2.70273
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C	3.39676	-1.92507	-1.14462
H	2.37888	-2.29969	-0.97143
C	4.24775	3.02343	-0.37863
H	3.61604	3.72458	-0.94237
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C	-3.85516	-0.22948	-1.19129
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H	1.02497	3.4093	-0.28737
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H	4.80151	-1.97063	-2.83036
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C	-1.55099	3.58031	-1.43648
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H	4.33398	-3.73356	-0.40928
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H	3.99236	-2.51747	0.84951
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H	1.61994	-1.56689	3.01055
H	0.16728	-1.1719	3.97826
C	0.40462	-3.52208	1.41343
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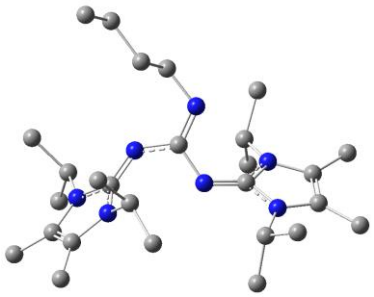

2b

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C	2.71317	-2.2275	1.03441
H	1.70829	-1.96388	1.3885
C	-3.02615	-2.24943	-0.31007
C	-1.2936	2.63441	2.44745
H	-1.86249	1.71313	2.23553
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H	-1.06258	3.1239	0.36858
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C	2.23089	1.87992	-1.59987
H	1.16074	1.72001	-1.44067

C	4.39249	-0.63612	-0.11184
C	2.4855	1.63856	-3.08789
H	3.52585	1.82895	-3.3829
H	1.84699	2.31216	-3.67726
H	2.23204	0.60325	-3.35596
C	-3.01434	0.78218	-2.33835
H	-2.0926	1.36522	-2.21118
C	-3.37695	-3.6292	0.13872
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H	-3.63499	-3.67359	1.20609
C	4.25104	0.55106	-0.75829
C	-0.75273	-2.97439	1.80278
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H	-2.07884	-1.38279	3.6734
H	-3.33313	-2.11514	2.64443
C	3.5772	-2.53279	2.25494
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H	3.59537	3.57148	-1.34489
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H	2.19251	-4.29569	0.62847
H	3.54443	-3.68775	-0.3588
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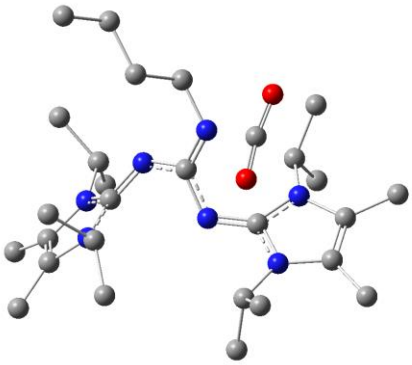

TS2b-3b

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C	1.65382	-1.194	-1.93443
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C	-2.32698	-2.33322	-1.25883
H	-1.38344	-1.86627	-1.56849
C	3.474	-2.07154	-0.36292
C	-2.45711	1.89169	-1.53554
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C	0.17837	2.99035	-0.29404

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C	-2.1521	0.32927	3.70766
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H	4.86442	-3.62109	-0.80063
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C	2.5586	-0.53483	-2.97348
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H	1.99993	-0.37413	-3.90646
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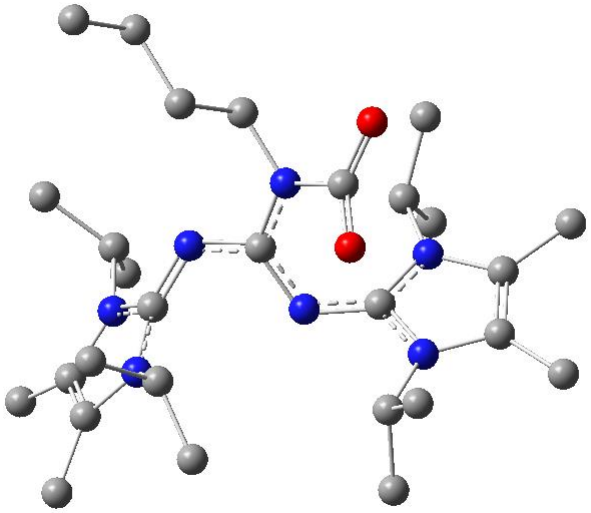

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C	-1.89573	-0.55691	0.4695
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C	2.17291	-0.3855	0.24847
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C	-2.36622	-2.37384	-1.11079
H	-1.37508	-1.99616	-1.38629
C	3.41909	-2.22693	-0.09683

C	-1.86476	1.61717	-1.36683
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C	3.94518	-1.57195	0.97528
C	0.1117	2.95245	-0.54814
H	0.80238	2.99475	0.30694
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H	-6.0637	-1.77706	0.77726

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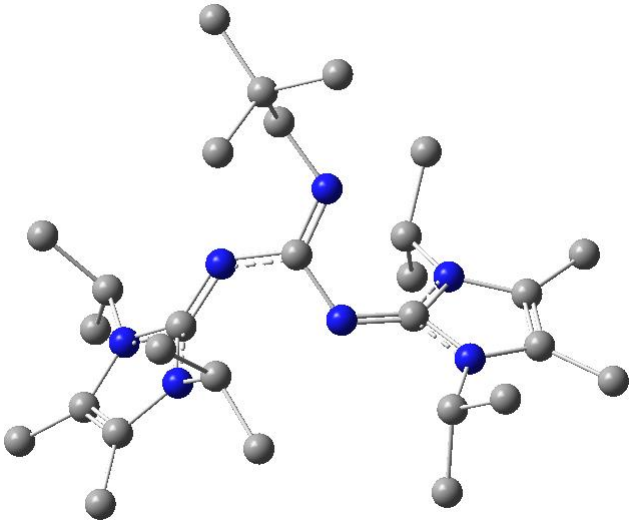

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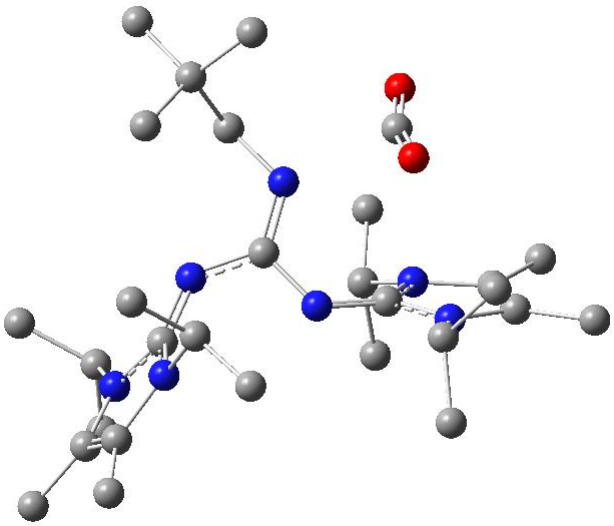

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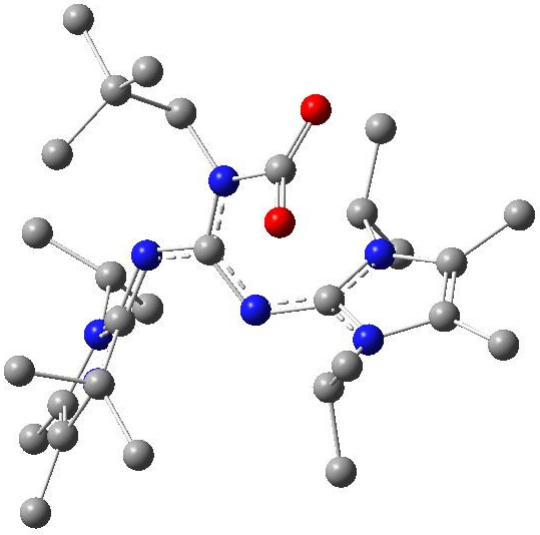

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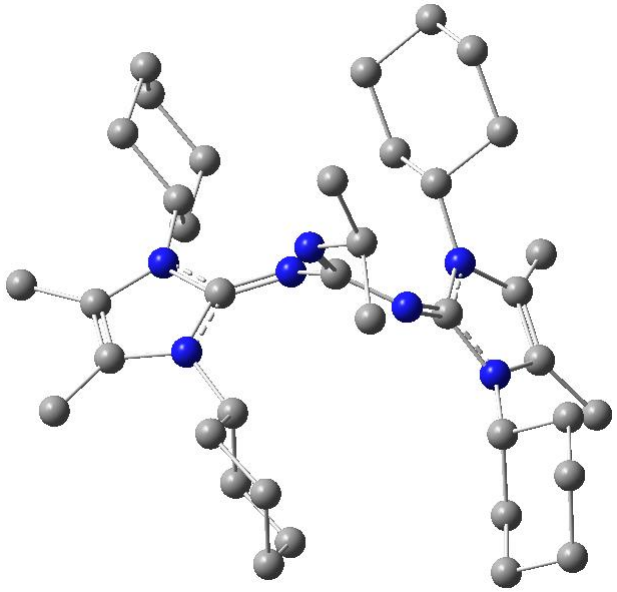

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H	5.1089	-1.10741	-3.10342
H	4.41827	-1.77498	-1.62113
H	6.85703	-0.05409	0.70952
H	5.44669	-1.11917	0.67021
H	6.86623	-1.48604	-1.34908
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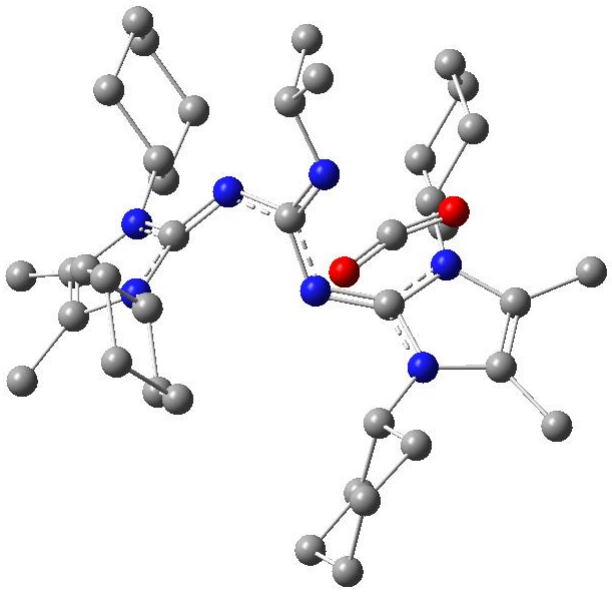

TS2d-3d

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N	0.84588	2.6147	-0.48025
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C	1.30874	1.32424	-0.48278

C	-0.18728	0.14679	0.85223
C	-1.5483	-1.53897	-0.08947
C	-1.43872	-3.5534	-1.10288
C	2.25812	1.1188	2.20507
C	-2.6692	-3.03486	-1.36104
C	2.9605	2.7184	-1.15301
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H	-0.04657	-4.62132	-2.35112
H	-1.61273	-5.42083	-2.11091
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C	1.8682	3.47873	-0.87756
C	1.77508	4.96851	-0.85049
H	2.63875	5.40153	-1.36855
H	0.86811	5.35104	-1.3357
H	1.78655	5.34031	0.18516
C	4.30213	3.1842	-1.61483
H	5.04099	3.20747	-0.80057
H	4.70038	2.54628	-2.41547
H	4.21513	4.20052	-2.01702
C	-3.7681	-3.61411	-2.18808
H	-4.73375	-3.57659	-1.66428
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H	-3.55048	-4.66632	-2.40493
C	0.18057	0.70798	4.40598
H	-0.40126	0.51599	5.31948
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H	0.53493	1.74999	4.42946
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H	-2.52417	1.15891	2.28123

H	-2.54451	1.10316	4.06498
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C	-4.81251	-1.34663	0.49547
H	-3.38469	0.06173	-0.22368
C	-5.66259	0.52966	-1.62008
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C	-5.90691	-0.30892	0.74529
H	-5.26781	-2.30479	0.18845
H	-4.23446	-1.53451	1.41271
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C	1.68503	-3.24013	-0.29918
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C	1.36396	-3.95488	2.5593
H	-0.0816	-4.85588	1.21904
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C	2.6253	-4.32489	1.77836
H	1.17413	-4.68499	3.36001

H	1.51787	-2.97604	3.04484
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H	3.06722	-2.32998	1.08512
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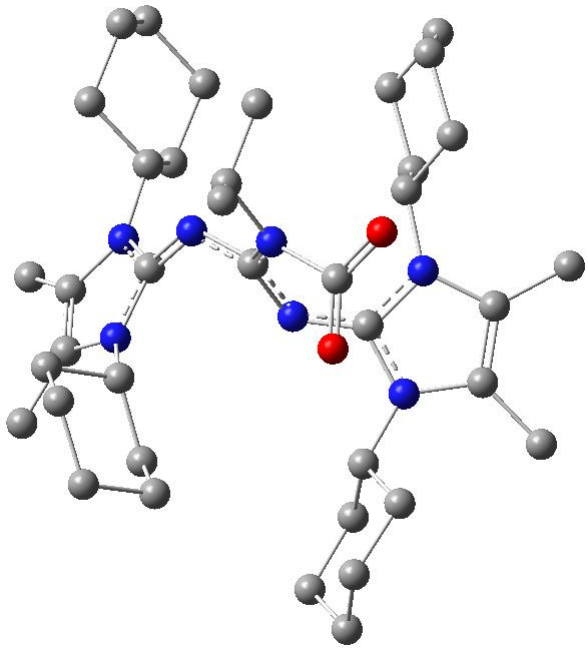

3d

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C	-0.98939	-3.76273	-0.99383
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H	0.53942	-4.71683	-2.17119
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C	1.19231	5.05005	-1.27016
H	1.93661	5.46311	-1.96124
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C	-5.83328	-0.71017	0.33429
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H	0.5231	-4.92015	1.38437
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