

Carbon Dioxide Hydrogenation to Formate Catalyzed by Highly Active Ru-tris(pyrazolyl)methane Complexes

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SUPPORTING INFORMATION

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 - 3.2 Screening of the effects of catalyst concentration, pressure, temperature, reaction time and addition of a Lewis acid on CO₂ Hydrogenation
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1. General Methods and Materials

For the synthesis of the complexes, reactants and solvents were purchased from Merck, Strem or TCI Chemicals, and were of the highest purity available. Complexes **1-5** [1] and **7** [2] were prepared according to the respective literature procedures. Reactions were conducted under N₂ atmosphere using standard Schlenk techniques, and all products were stored in air once isolated. Solvents were used as received unless otherwise stated. Toluene and diethyl ether were dried with the solvent purification system mBraun MB SPS5, while methanol was distilled from calcium hydride and isopropanol from magnesium. IR spectra of solid samples were recorded on Agilent Cary630 FTIR spectrometer. NMR spectra were recorded at 298 K on a Jeol JNM-ECZ400S or JNM-ECZ500R instrument equipped with a Royal HFX Broadband probe. Chemical shifts (expressed in parts per million) are referenced to the residual solvent peaks (¹H, ¹³C) or to external standard (³¹P to H₃PO₄) [3]. ¹H and ¹³C{¹H} NMR spectra of ruthenium complexes were assigned with the assistance of ¹H-¹³C (*gs*-HSQC and *gs*-HMBC) correlation experiments [4]. Elemental analyses were performed on a Vario MICRO cube instrument (Elementar).

For the catalytic experiments, all manipulations were carried out using standard Schlenk and glovebox techniques under nitrogen atmosphere. A H₂/CO₂ (1:1) gas mixture was purchased from Air Liquide and used as received. Solvents were freshly distilled over appropriate drying agents, collected over Linde type 3Å or 4Å molecular sieves under nitrogen, and degassed with nitrogen. Deuterated solvents for NMR measurements were purchased from commercial suppliers and stored onto activated 4Å molecular sieves under nitrogen before use. The ¹H, ¹³C{¹H}, and ³¹P{¹H} NMR spectra of the catalytic and mechanistic experiments were recorded on a Bruker AVANCE-250 spectrometer (operating at 250.13, 101.26, and 62.90 MHz, respectively), on a Bruker Avance II 300 spectrometer (operating at 300.13, 75.47, and 121.50 MHz, respectively) and a Bruker Avance II 400 spectrometer (operating at 400.13, 100.61, and 161.98 MHz, respectively) at room temperature. Peak positions were calibrated against the residual solvent resonance (¹H) or the deuterated solvent multiplet (¹³C). ³¹P{¹H} NMR were referenced to 85% H₃PO₄, with the downfield shift taken as positive.

2. IR and NMR spectra of ruthenium complexes 6 and 8-10.

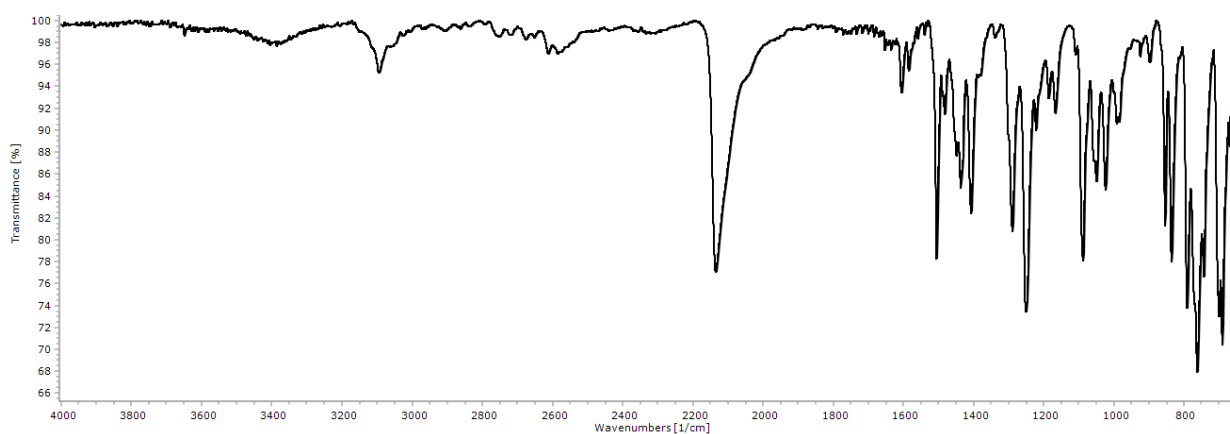


Figure S1. Solid-state IR spectrum (650-4000 cm⁻¹) of **6**.

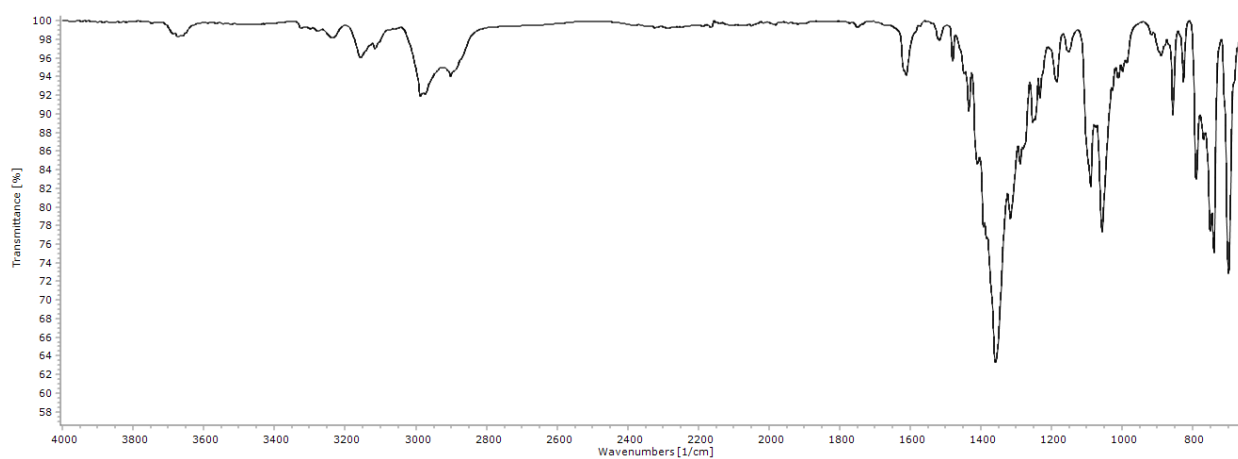


Figure S2. Solid-state IR spectrum (650-4000 cm⁻¹) of **8**.

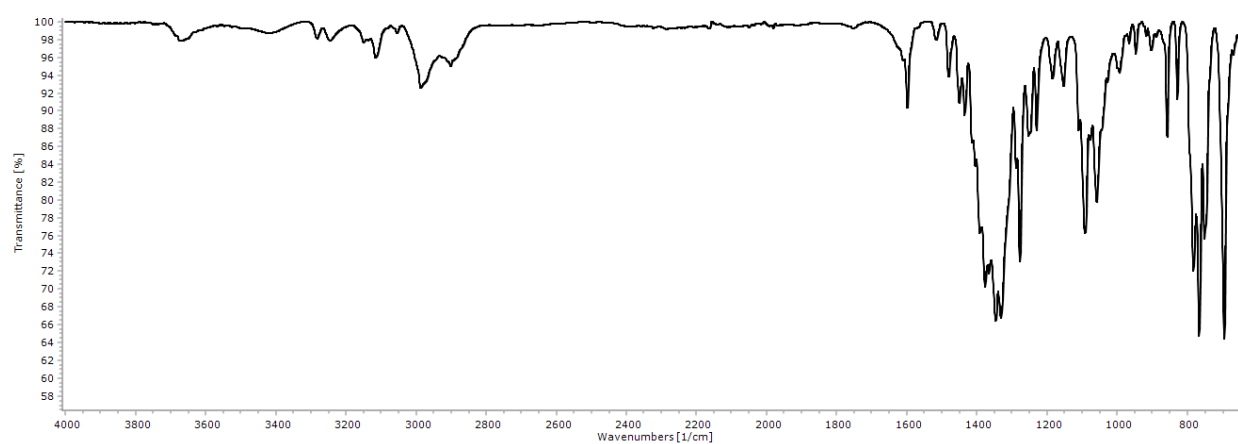


Figure S3. Solid-state IR spectrum (650-4000 cm⁻¹) of **9**.

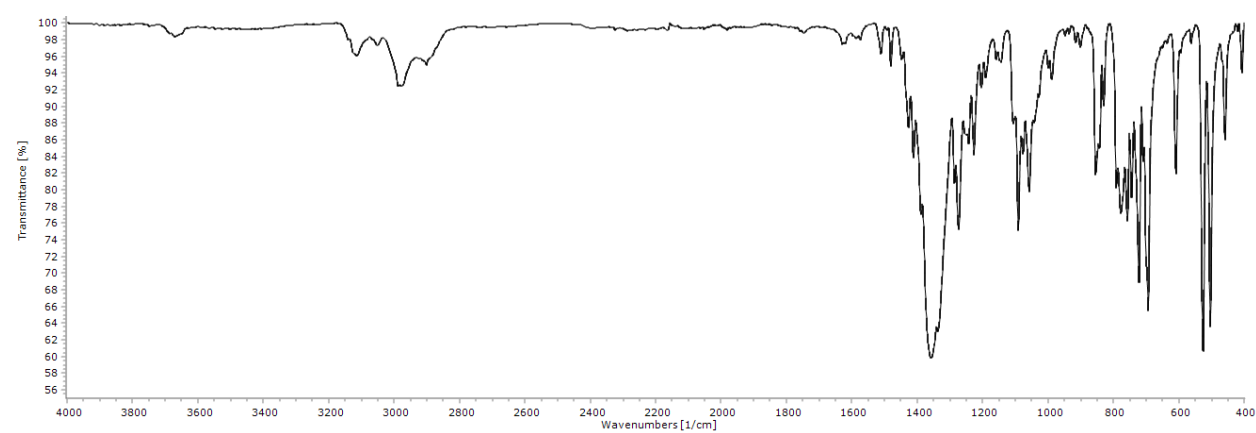


Figure S4. Solid-state IR spectrum (650-4000 cm⁻¹) of **10**.

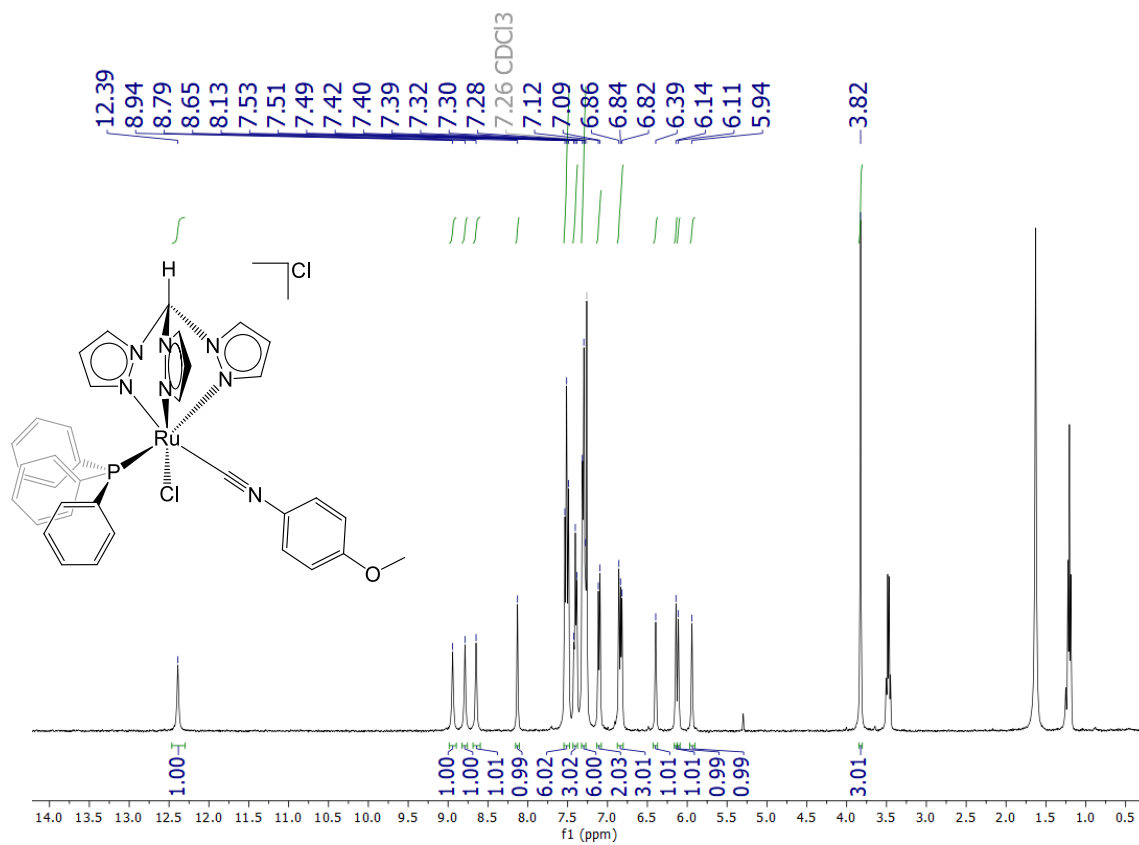


Figure S5. ^1H NMR spectrum (401 MHz, CDCl_3) of **6**.

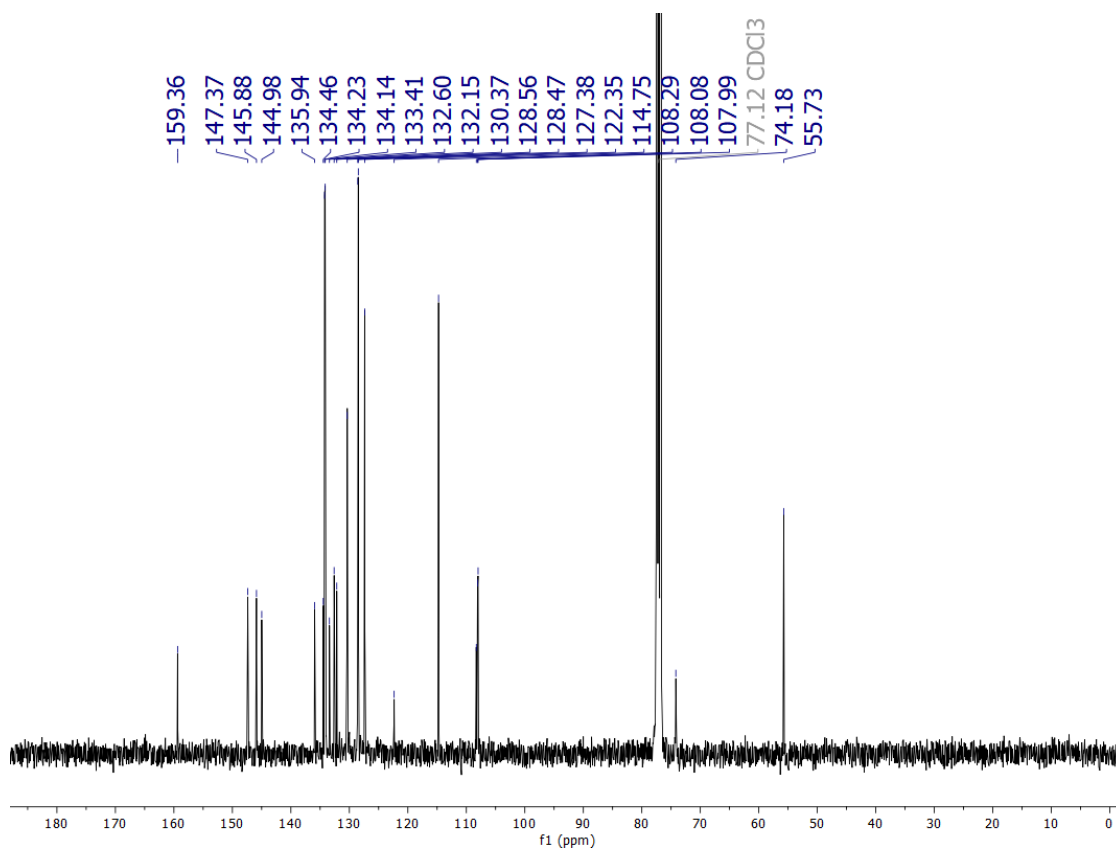


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **6**.

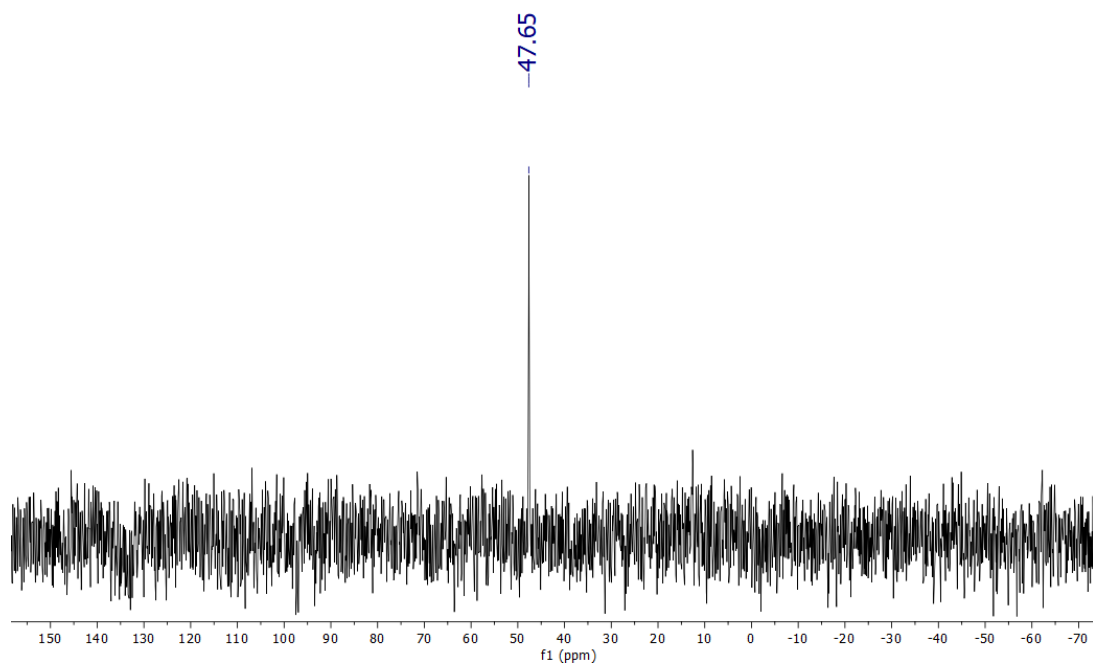


Figure S7. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (162 MHz, CDCl_3) of **6**.

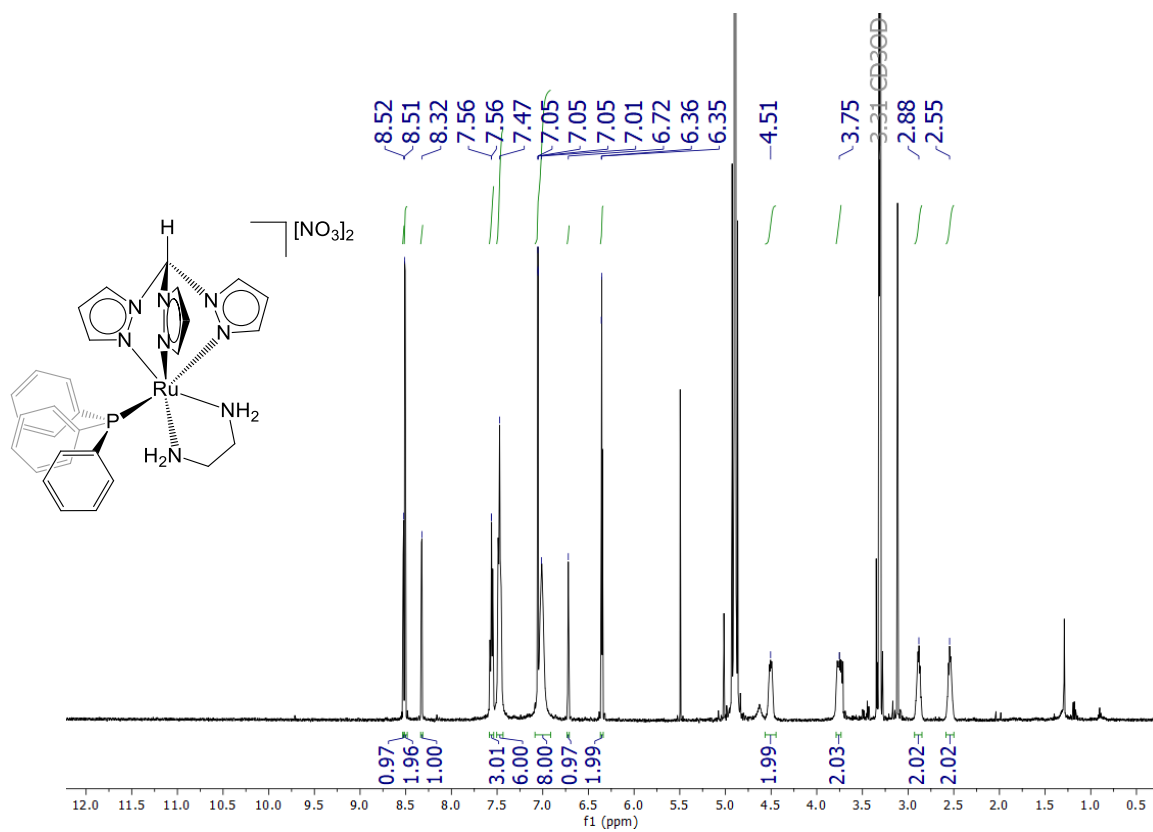


Figure S8. ^1H NMR spectrum (401 MHz, CD_3OD) of **8**.

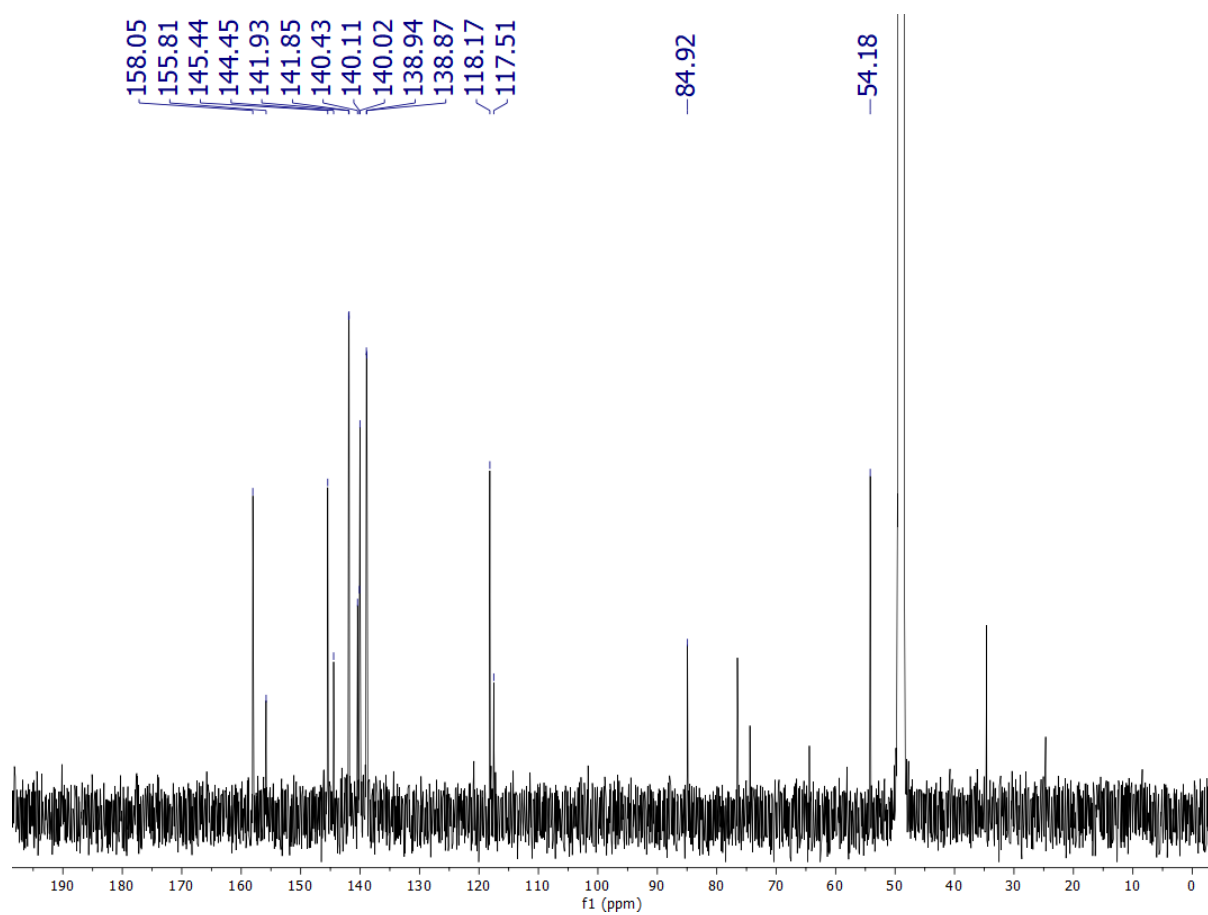


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CD_3OD) of **8**.

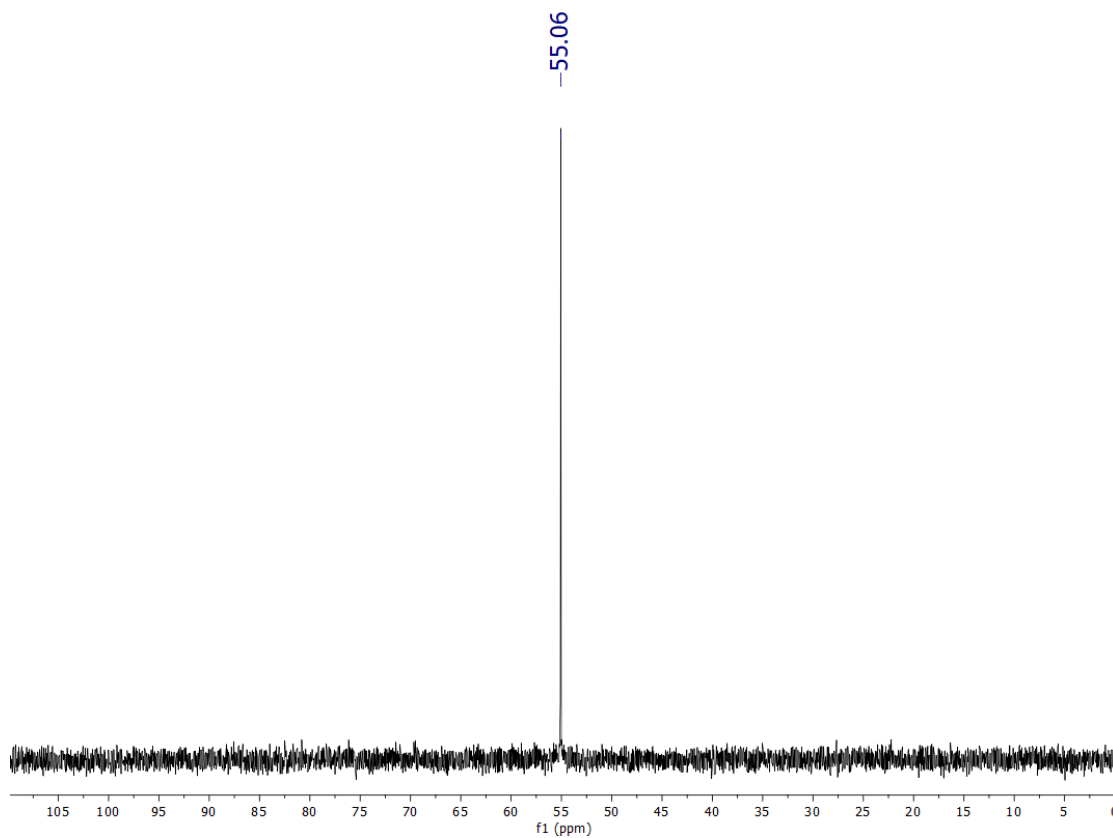


Figure S10. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (162 MHz, CD_3OD) of **8**.

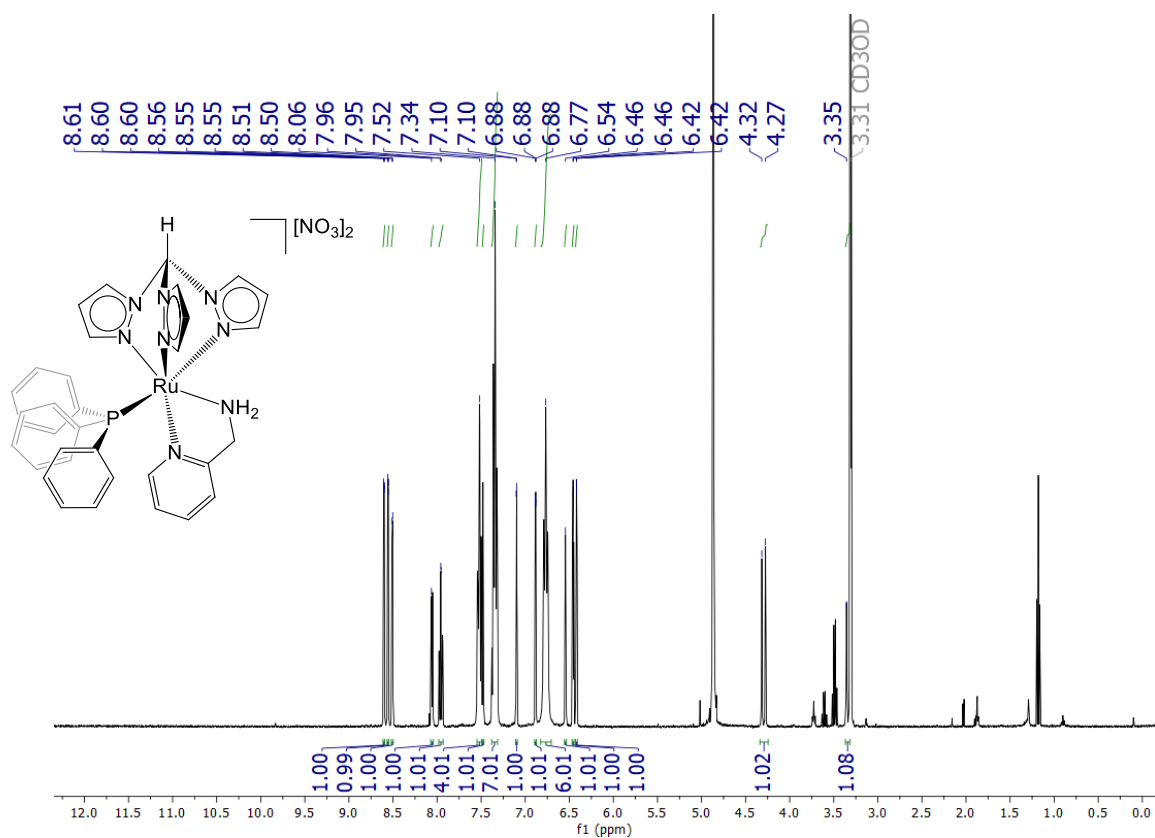


Figure S11. ^1H NMR spectrum (401 MHz, CD_3OD) of **9**.

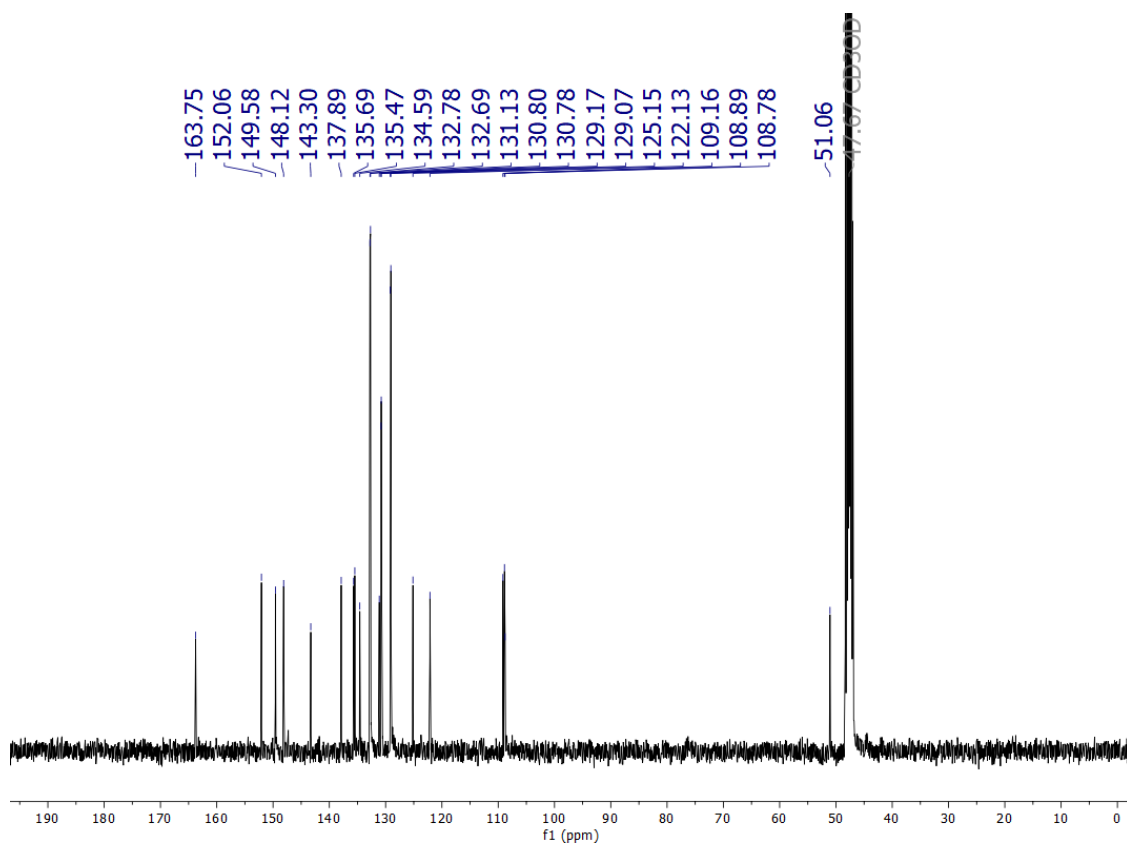


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CD_3OD) of **9**.

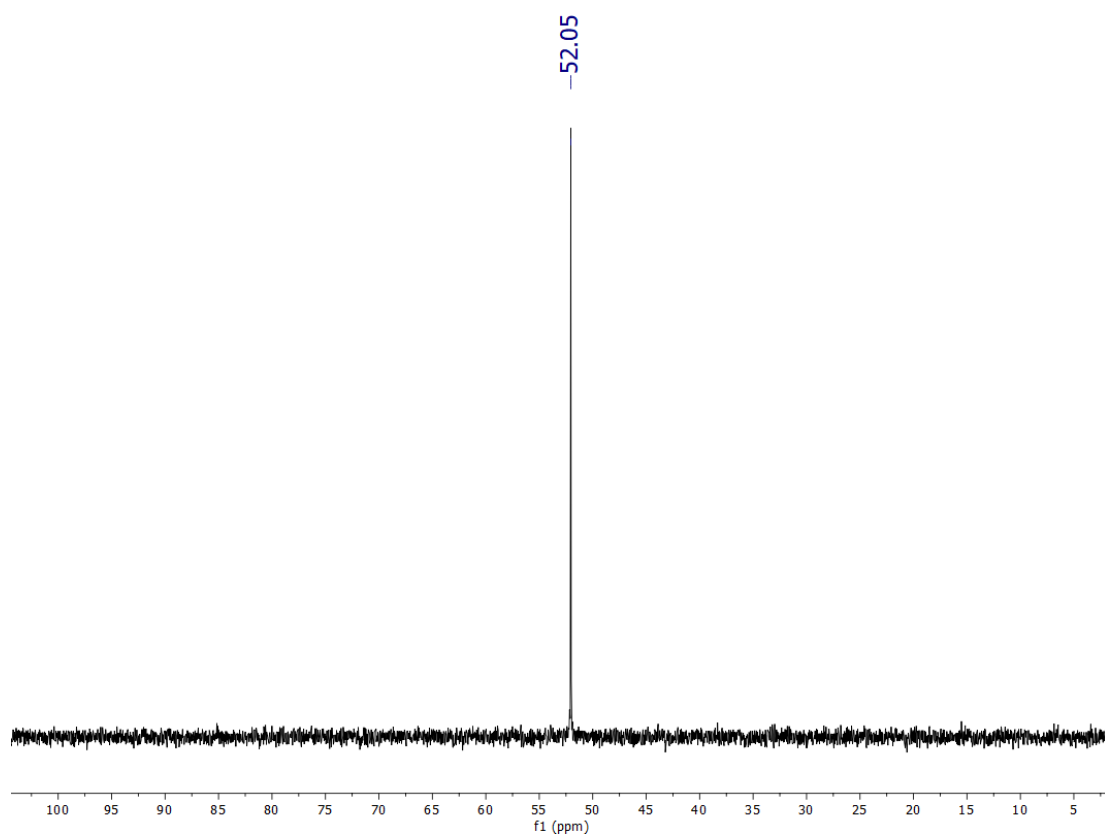


Figure S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (162 MHz, CD_3OD) of **9**.

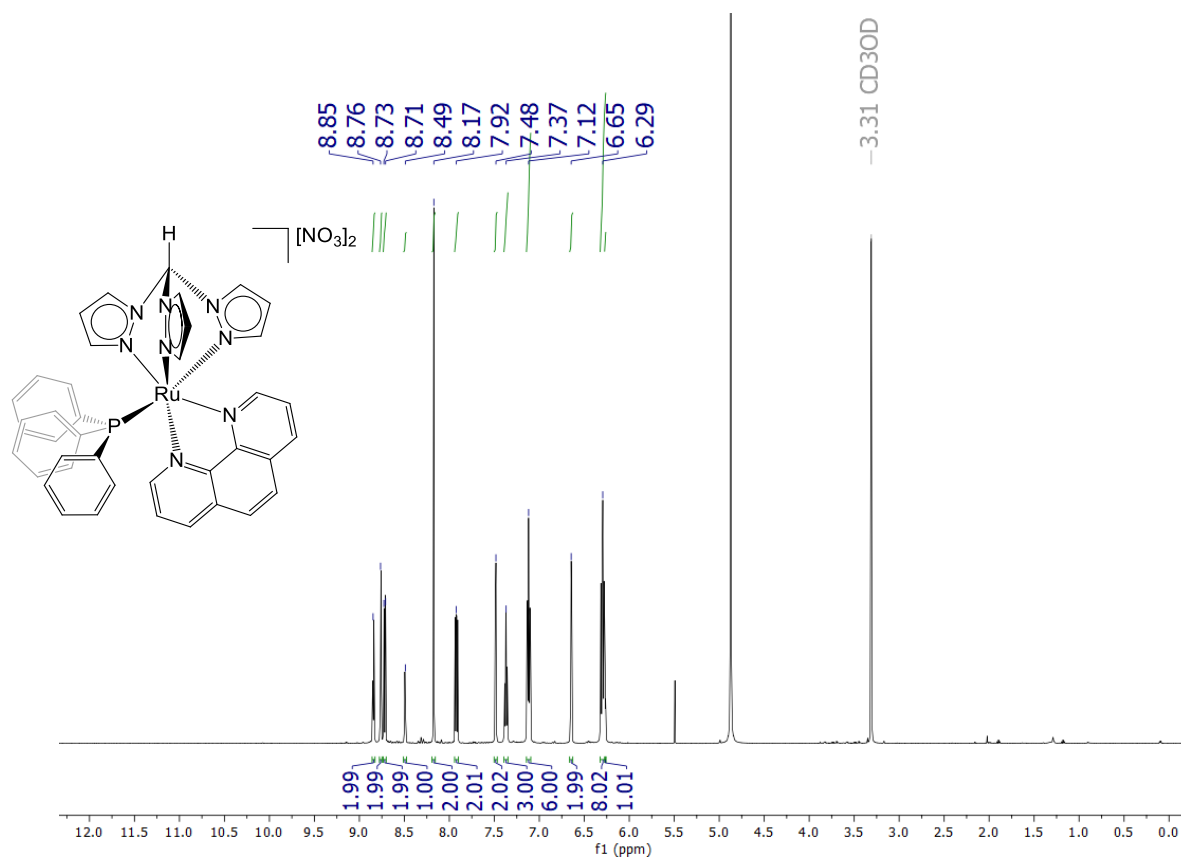


Figure S14. ^1H NMR spectrum (401 MHz, CD_3OD) of **10**.

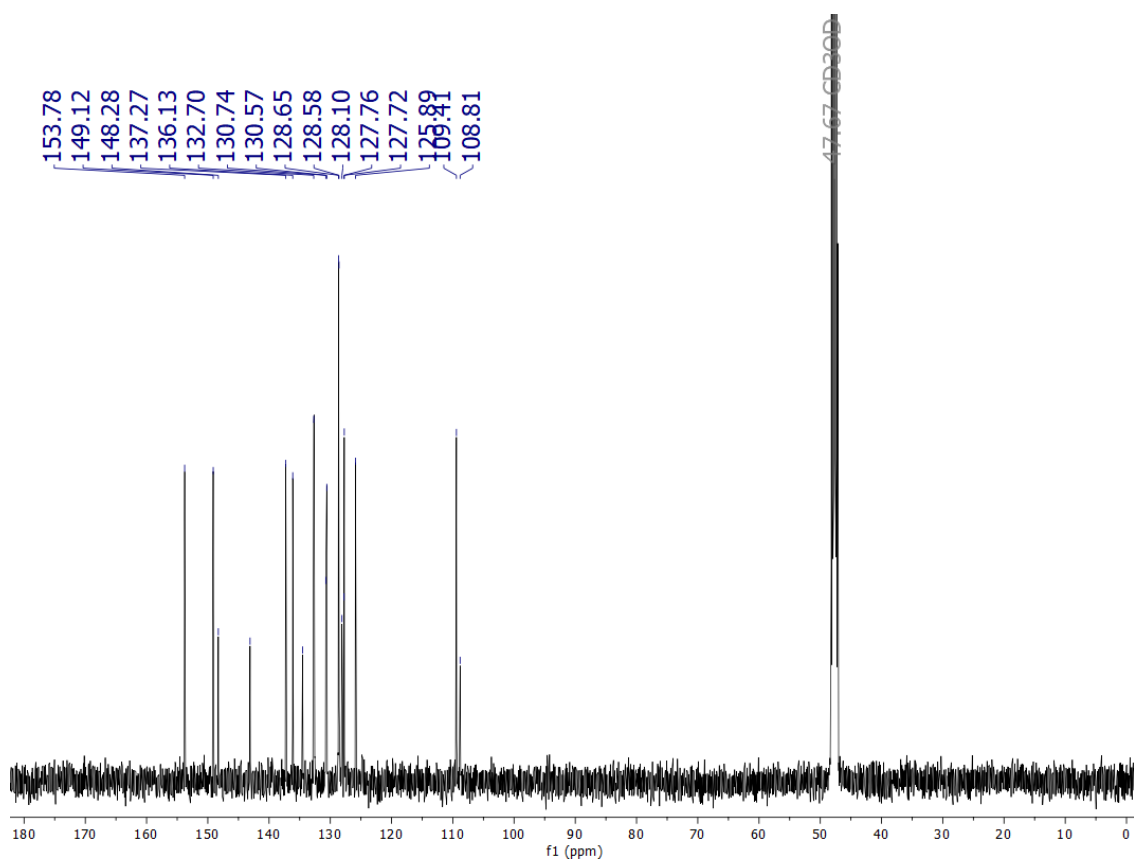


Figure S15. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (401 MHz, CD_3OD) of **10**.

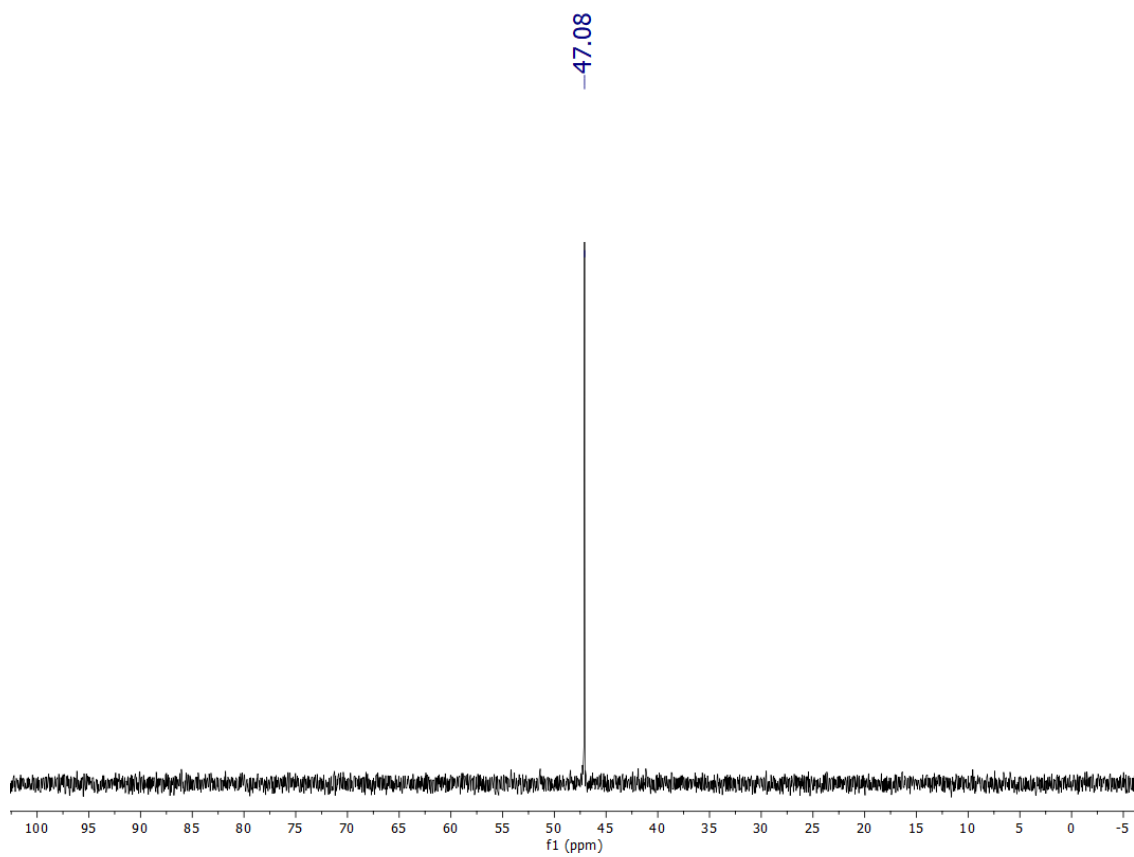


Figure S16. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (401 MHz, CD_3OD) of **10**.

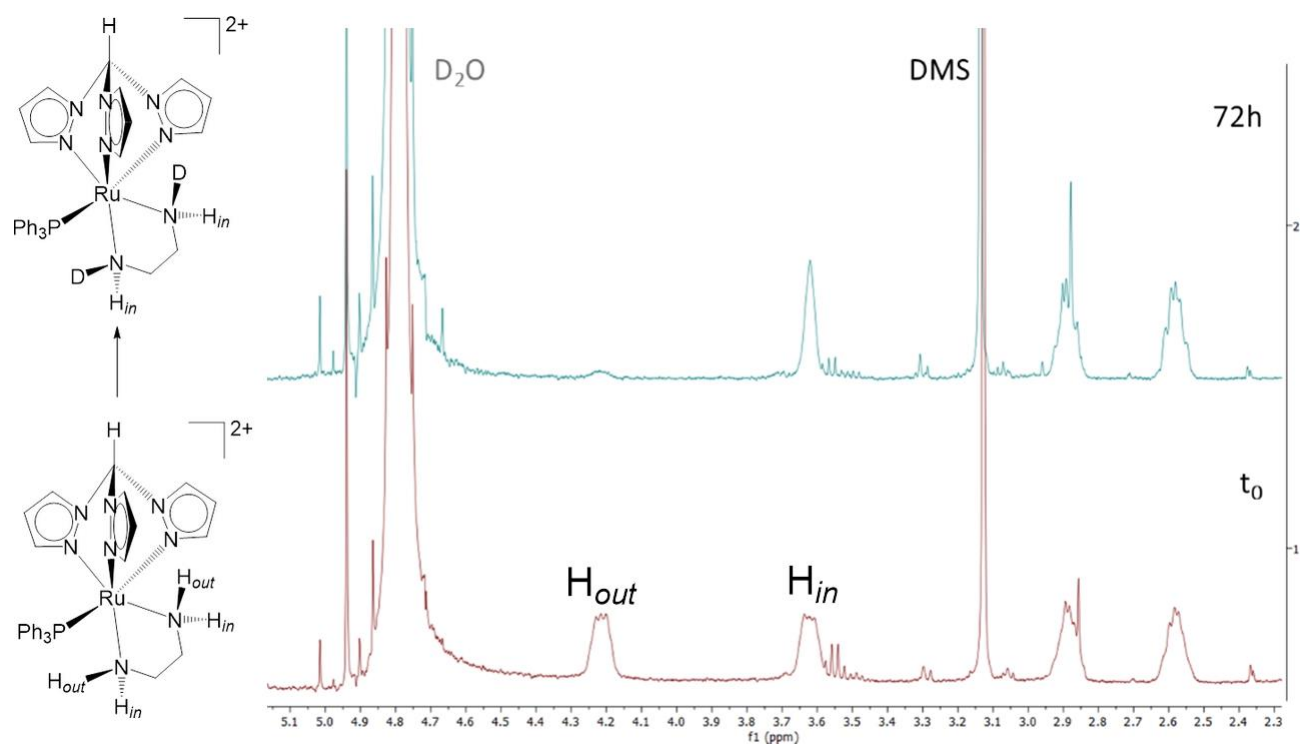


Figure S17. ^1H NMR spectra of **8** in D_2O immediately after preparation of the sample (bottom) and after 72 h (top).

3. ^1H NMR Spectra of Catalytic Runs

3.1. Screening of the effects of type of complexes and bases in CO_2 hydrogenation (Table 2 in main text)

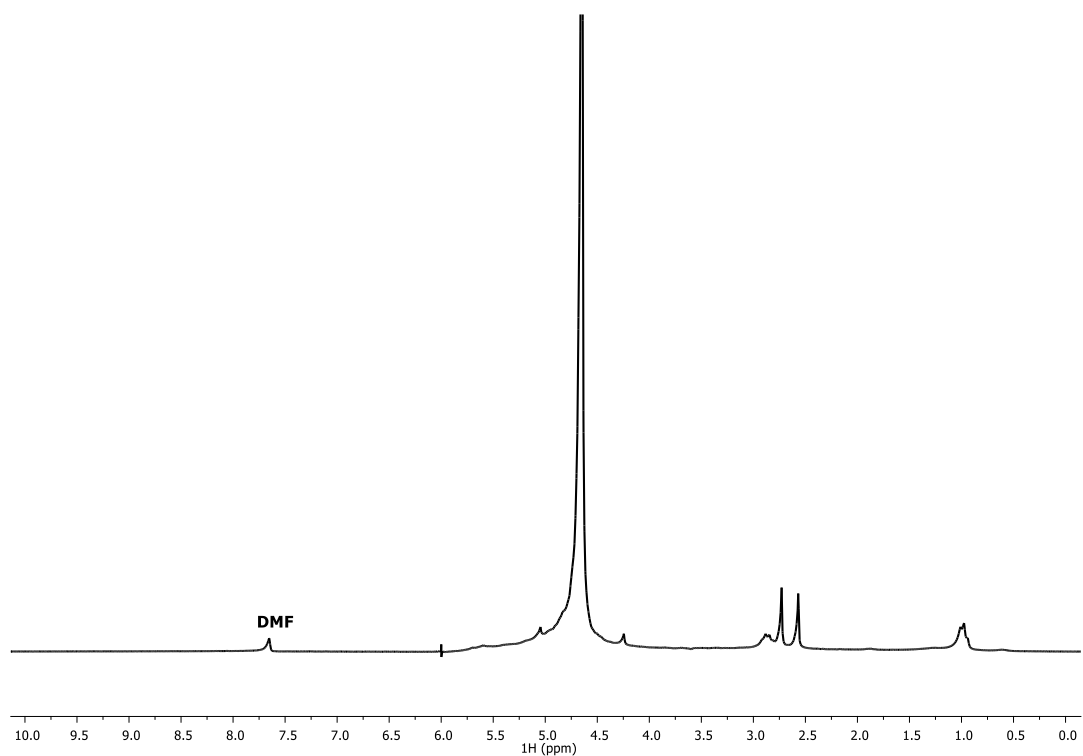


Figure S18. Conditions: $\mathbf{1}/\text{NEt}_3 = 1/1104$, THF, $p\text{H}_2/p\text{CO}_2$ (bar) = 30/30, 100 °C, 24 h (Entry 1).

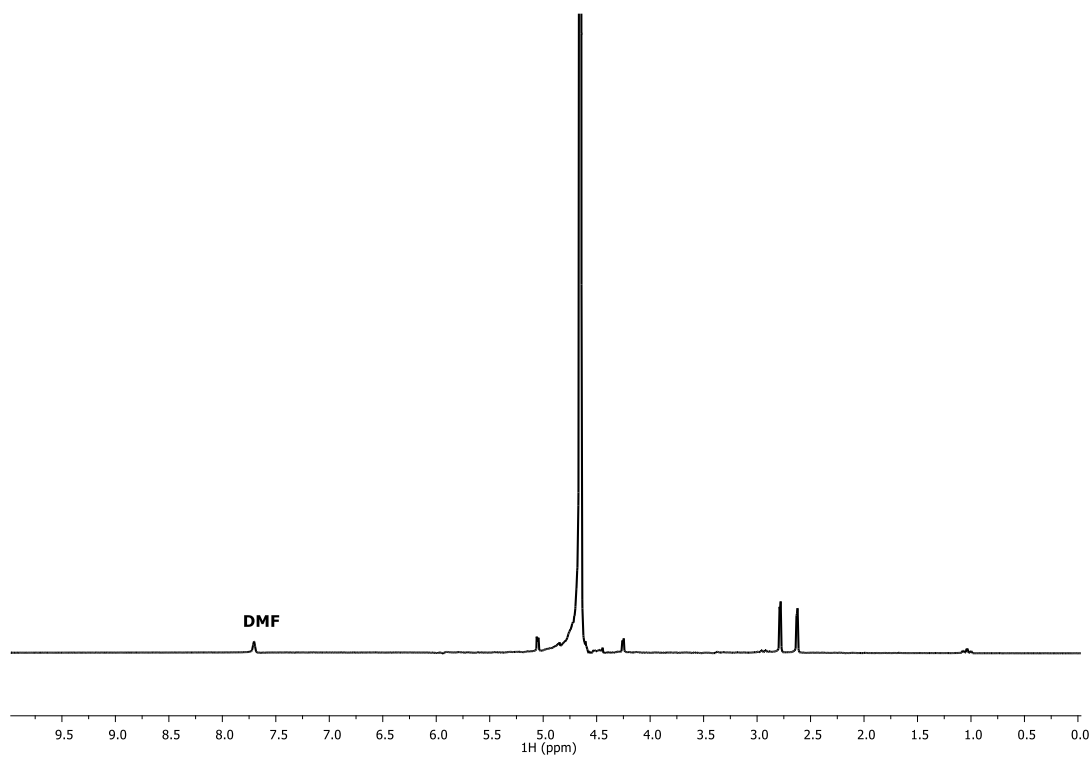


Figure S19. Conditions: $\mathbf{1}/\text{NEt}_3 = 1/1104$, THF/ H_2O , $p\text{H}_2/p\text{CO}_2$ (bar) = 30/30, 100 °C, 24 h (Entry 2).

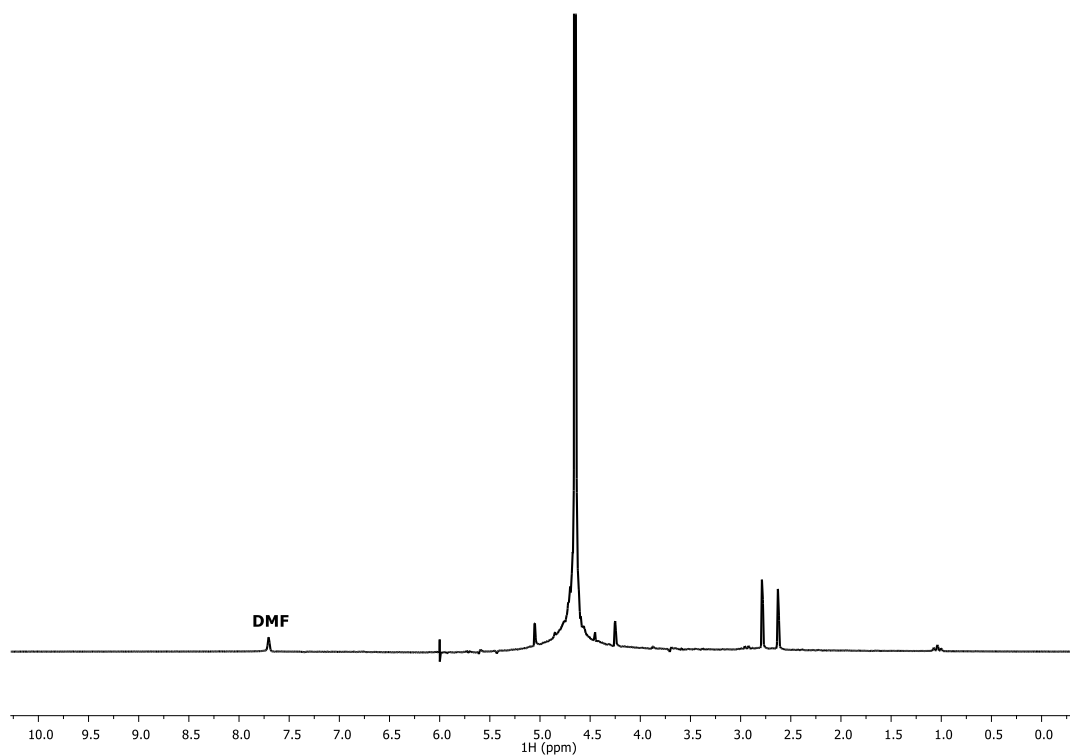


Figure S20. Conditions: **1**/NEt₃ = 1/1104, Toluene, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 3).

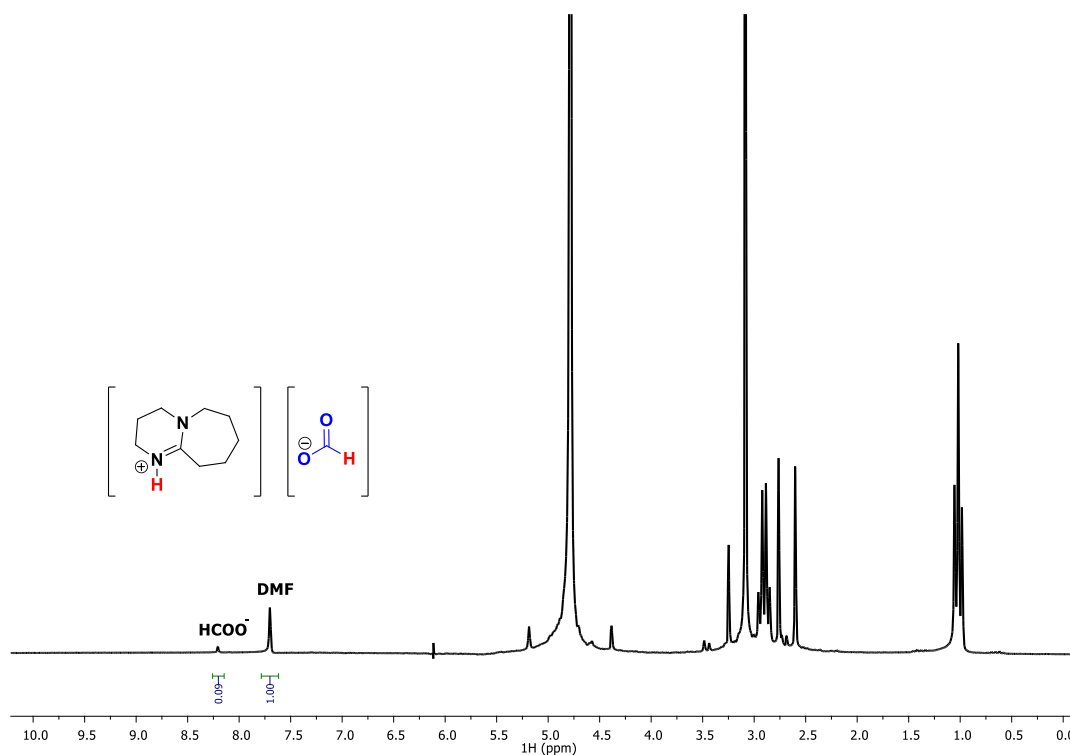


Figure S21. Conditions: **1**/NEt₃ = 1/1104, MeOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 4).

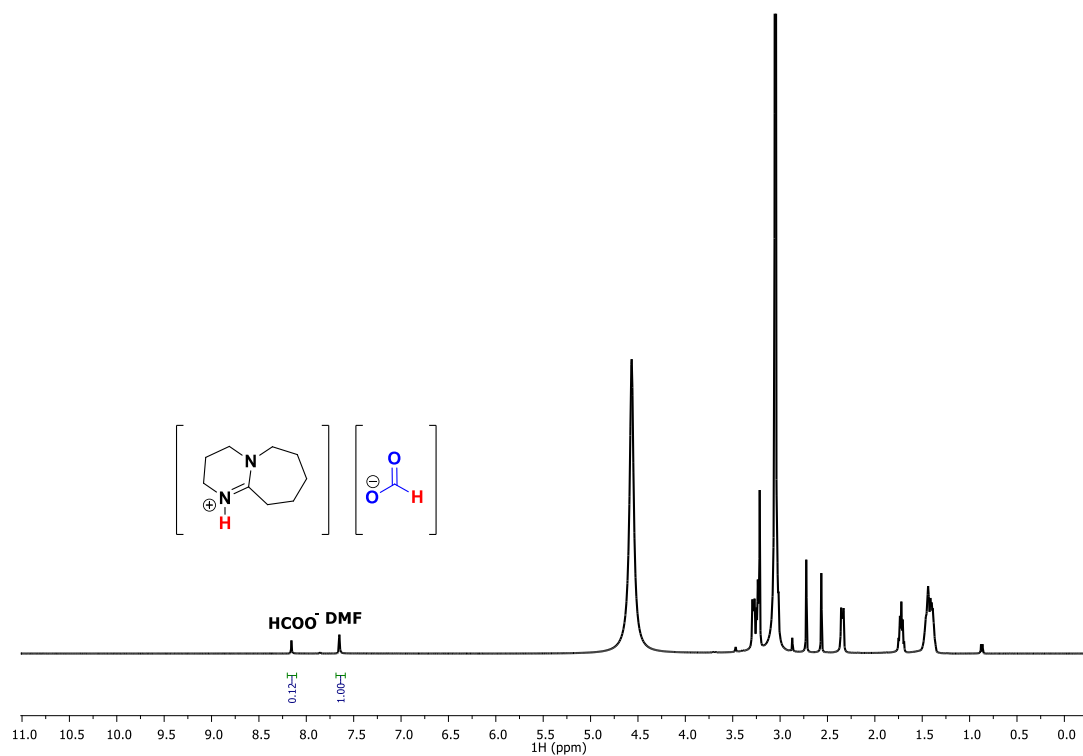


Figure S22. Conditions: **1**/DBU = 1/1000, MeOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 5).

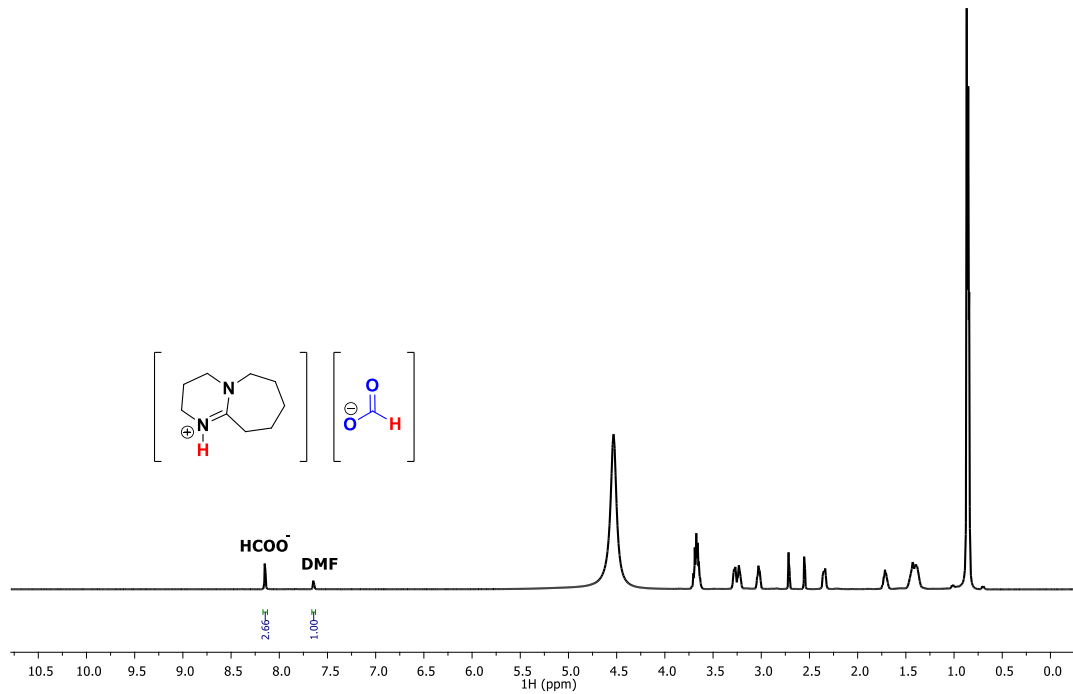


Figure S23. Conditions: **1**/DBU = 1/1000, ⁱPrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 6).

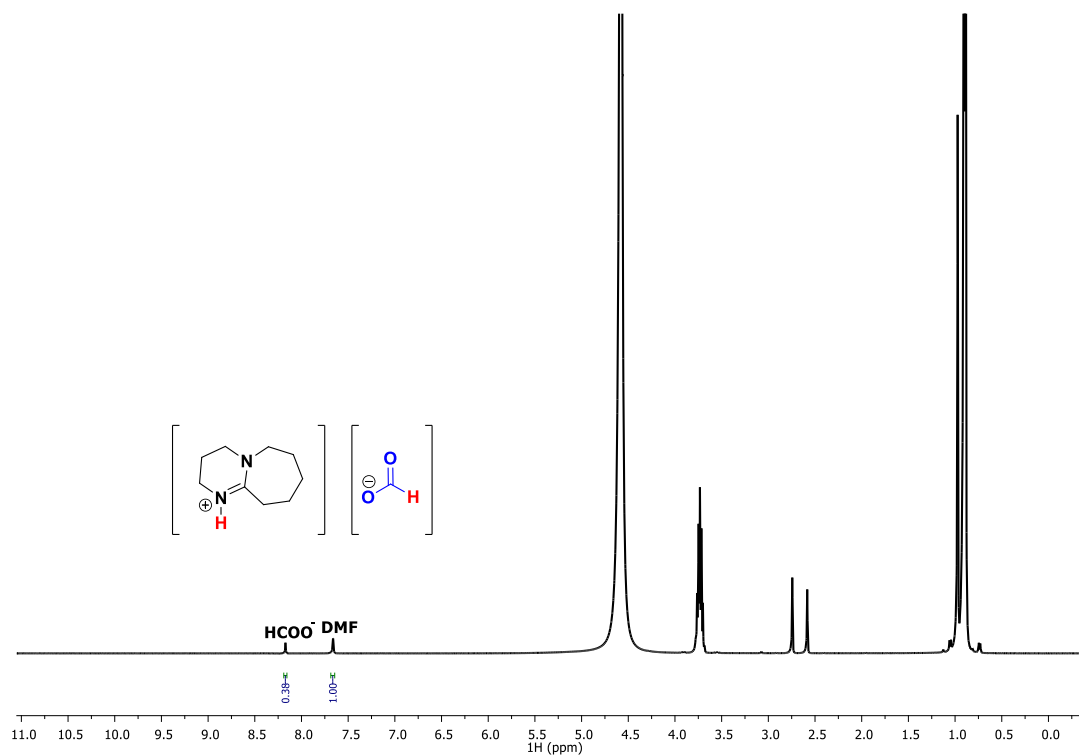


Figure S24. Conditions: **1**/KO^tBu = 1/1000, ⁱPrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 7).

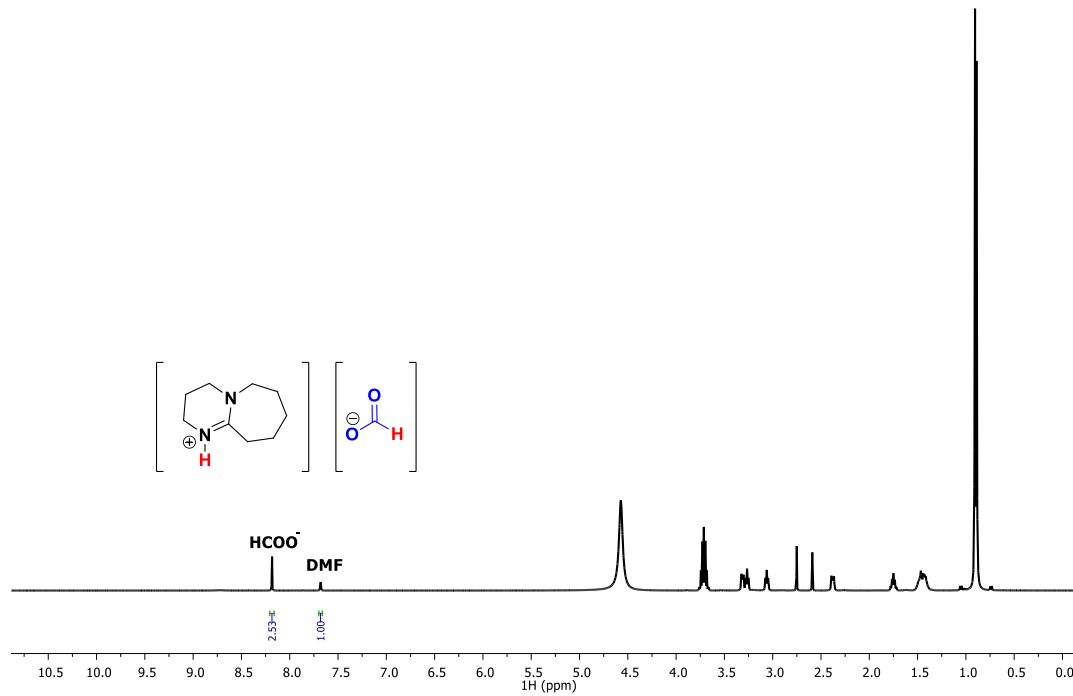


Figure S25. Conditions: **2**/DBU = 1/1000, ⁱPrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 8).

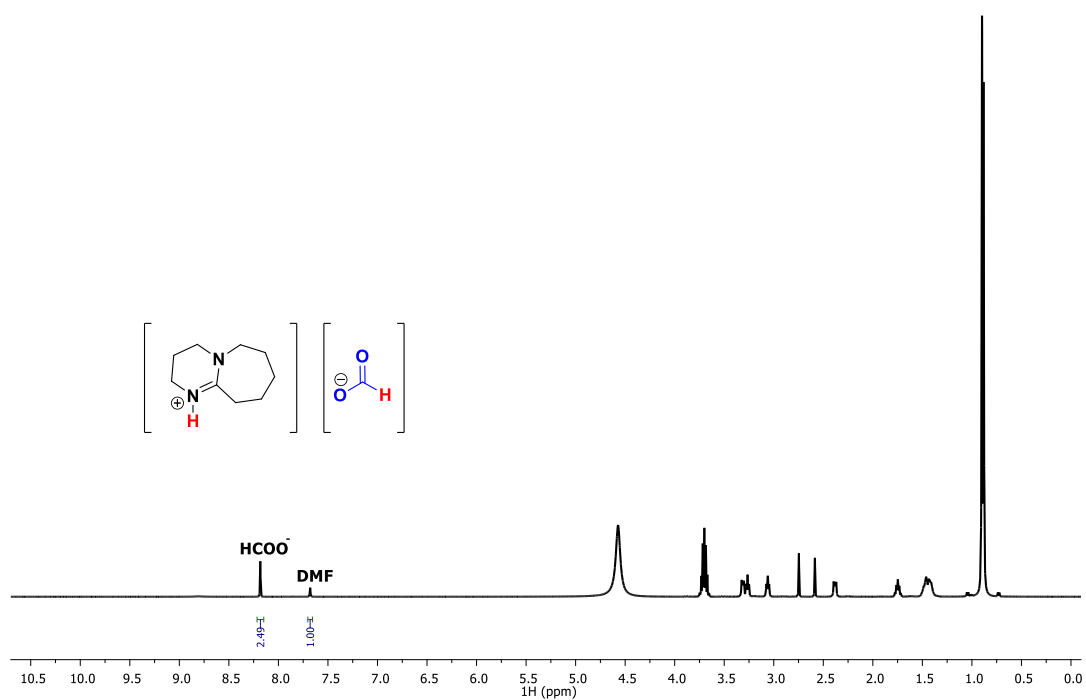


Figure S26. Conditions: **3**/DBU = 1/1000, ¹PrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 9).

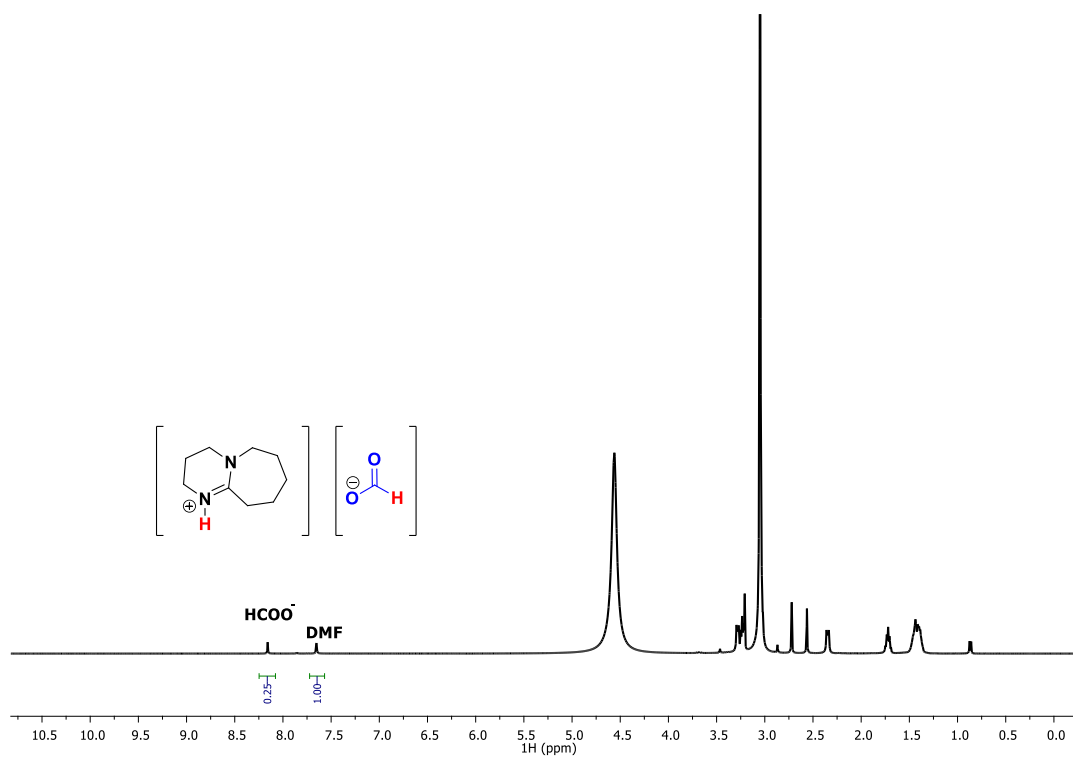


Figure S27. Conditions: **4**/DBU = 1/1000, MeOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 10).

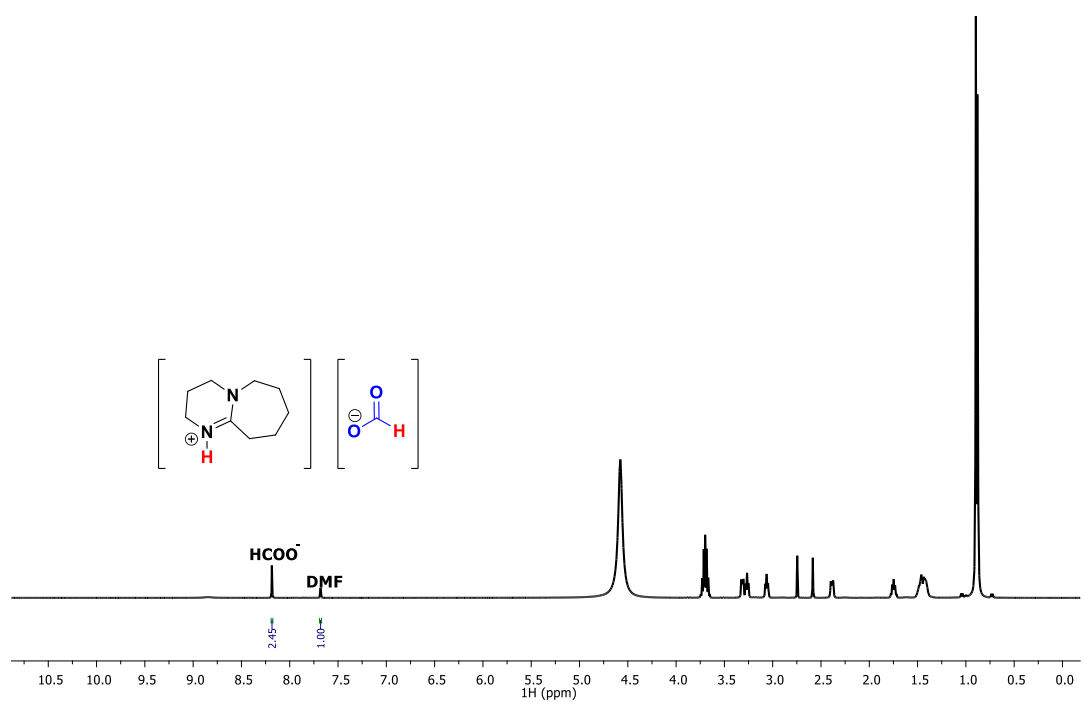


Figure S28. Conditions: **4**/DBU = 1/1000, ⁱPrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 11).

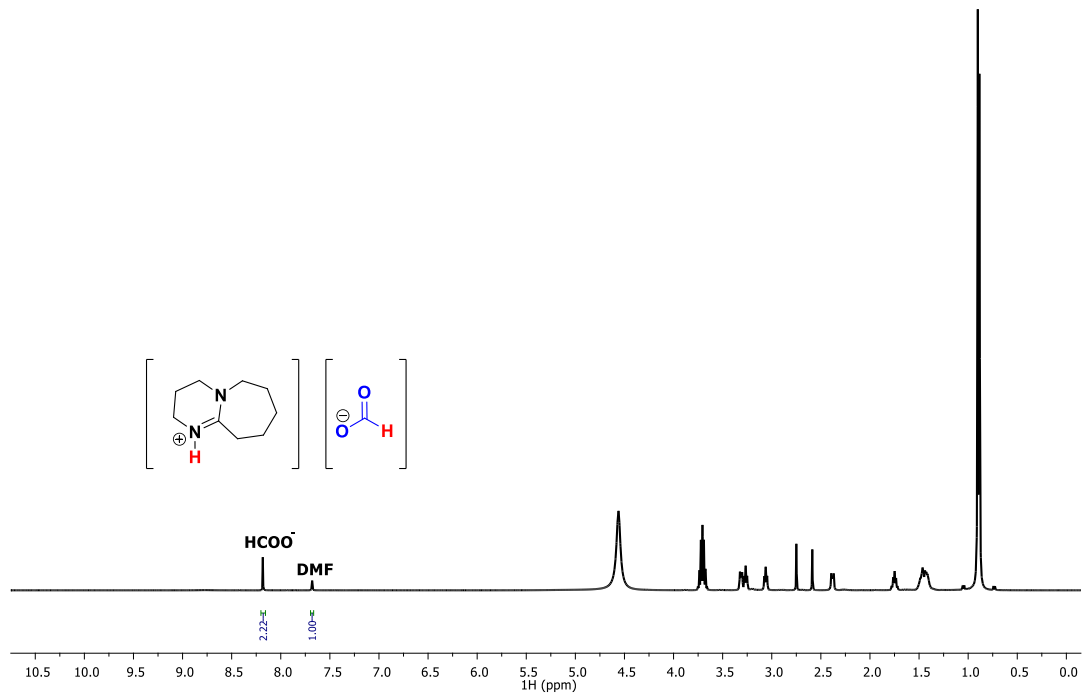


Figure S29. Conditions: **5**/DBU = 1/1000, ⁱPrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 12).

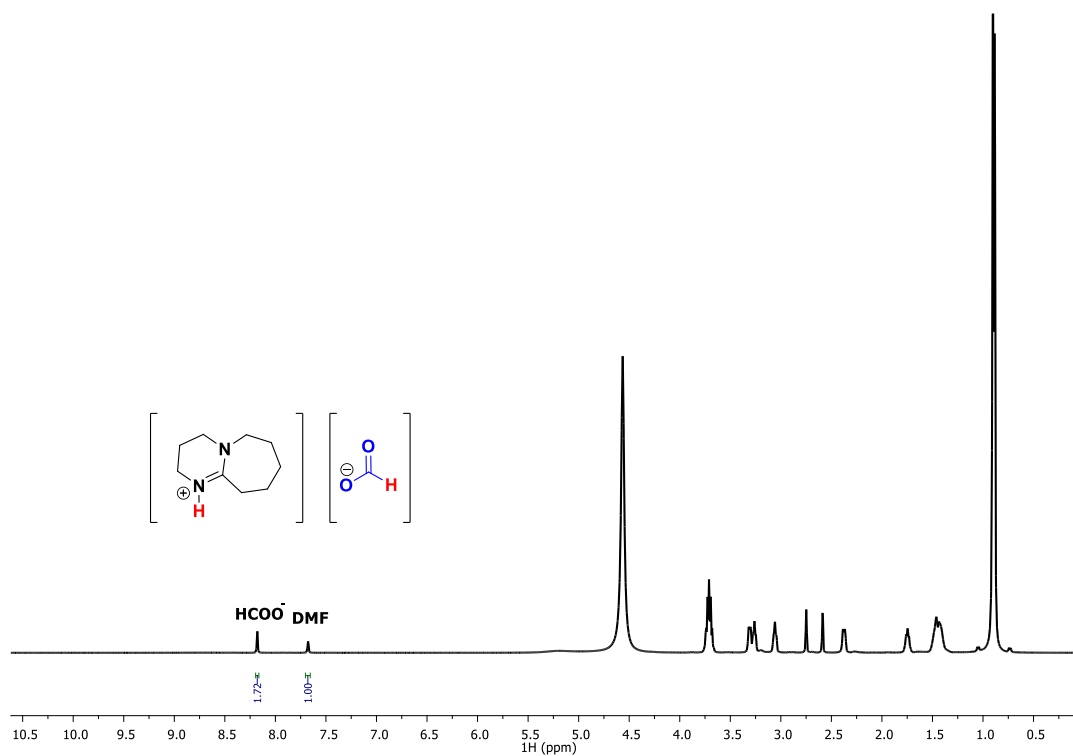


Figure S30. Conditions: **6**/DBU = 1/1000, ¹PrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 13).

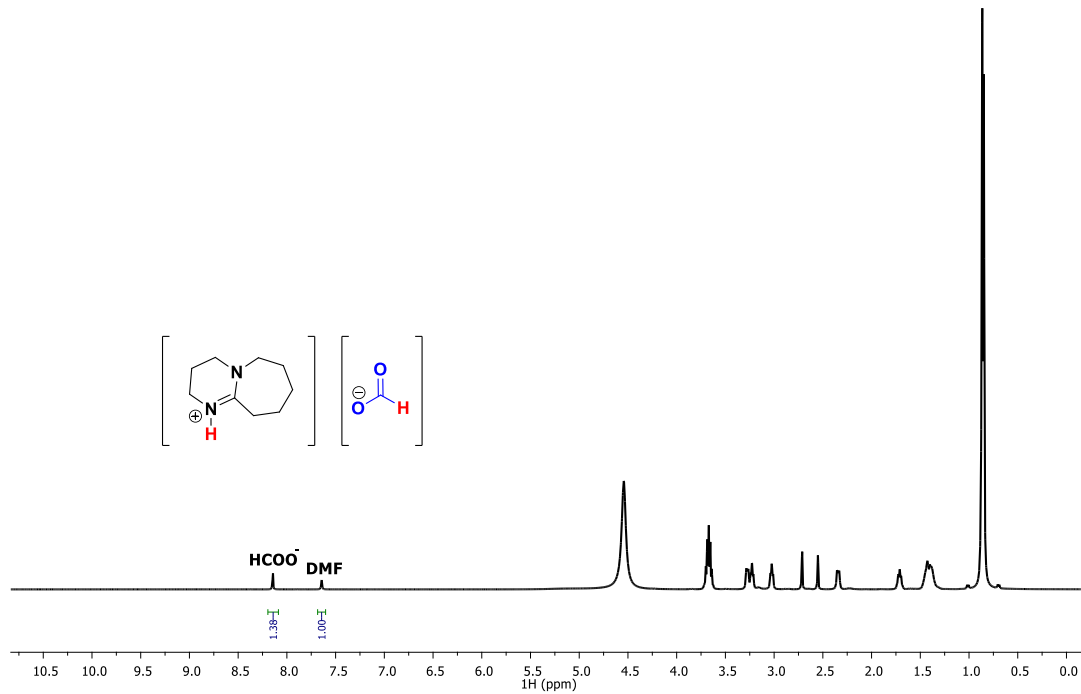


Figure S31. Conditions: **7**/DBU = 1/1000, ¹PrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 14).

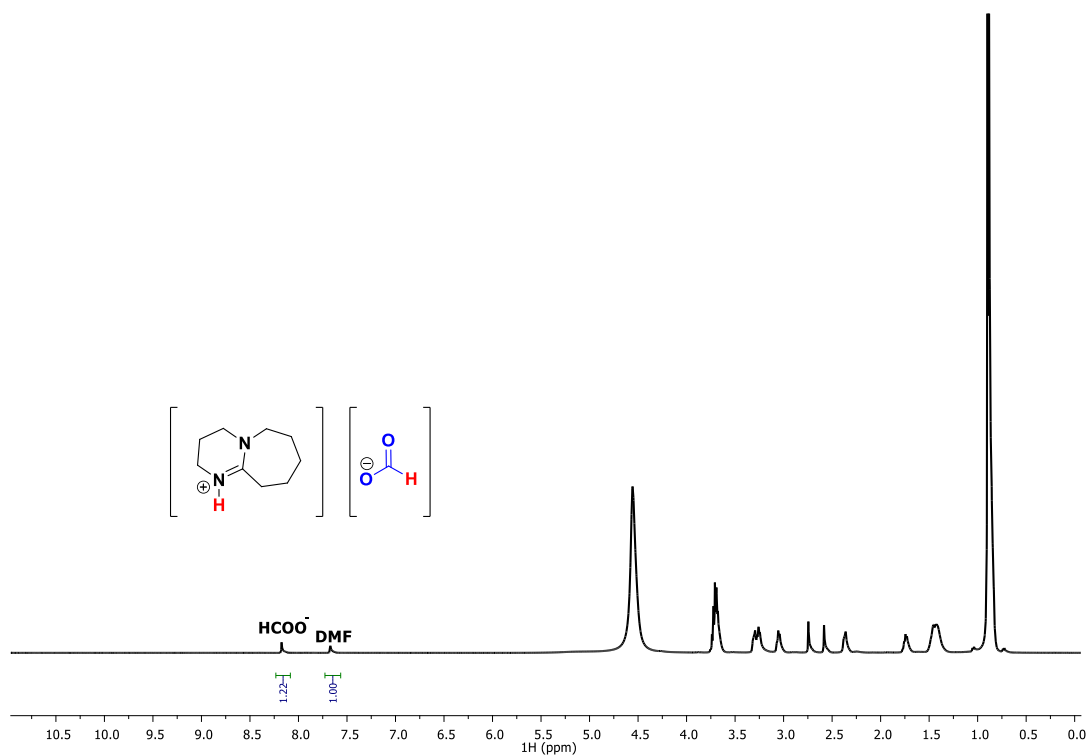


Figure S32. Conditions: **8**/DBU = 1/1000, ⁱPrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 15).

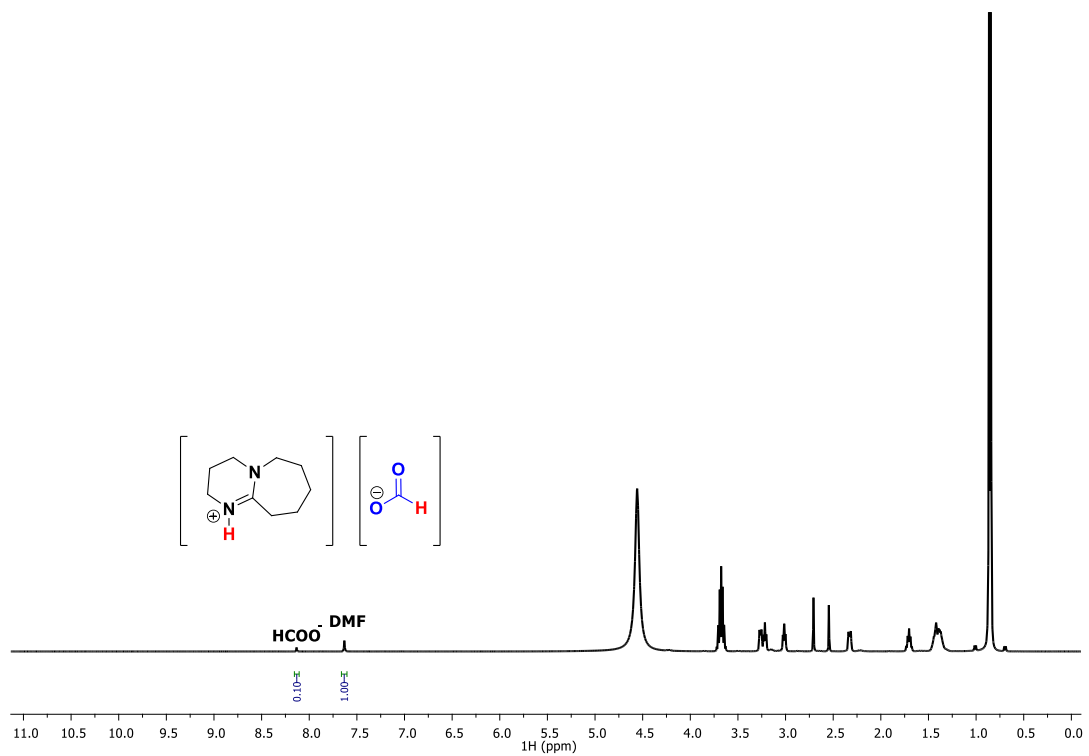


Figure S33. Conditions: **9**/DBU = 1/1000, ⁱPrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 16).

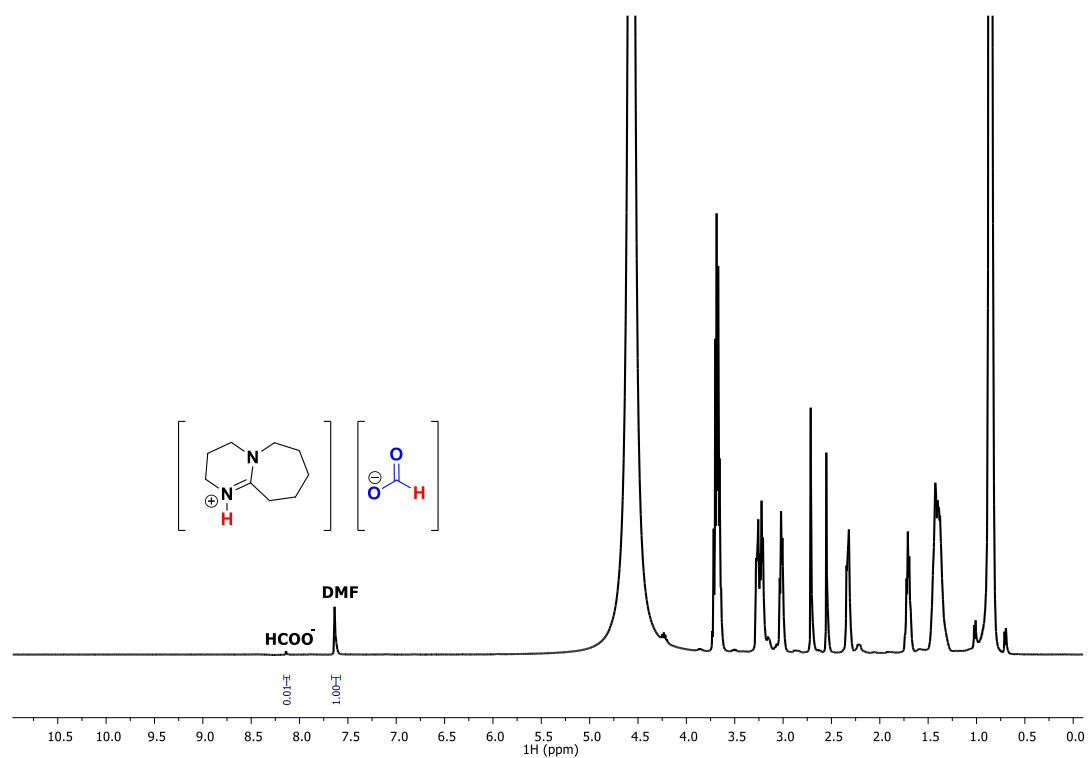


Figure S34. Conditions: **10**/DBU = 1/1000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 17).

3.2. Screening of the effects of catalyst concentration, pressure, temperature, reaction time and addition of a Lewis acid on CO₂ Hydrogenation (Table 3 in main text).

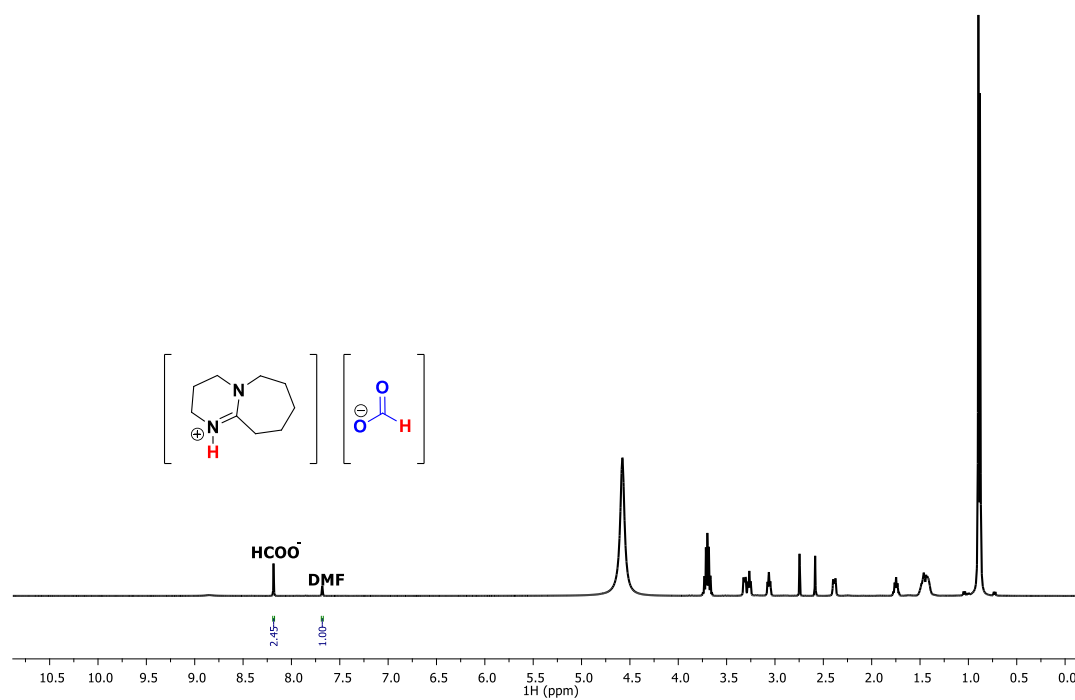


Figure S35. Conditions: **4**/DBU = 1/1000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 1).

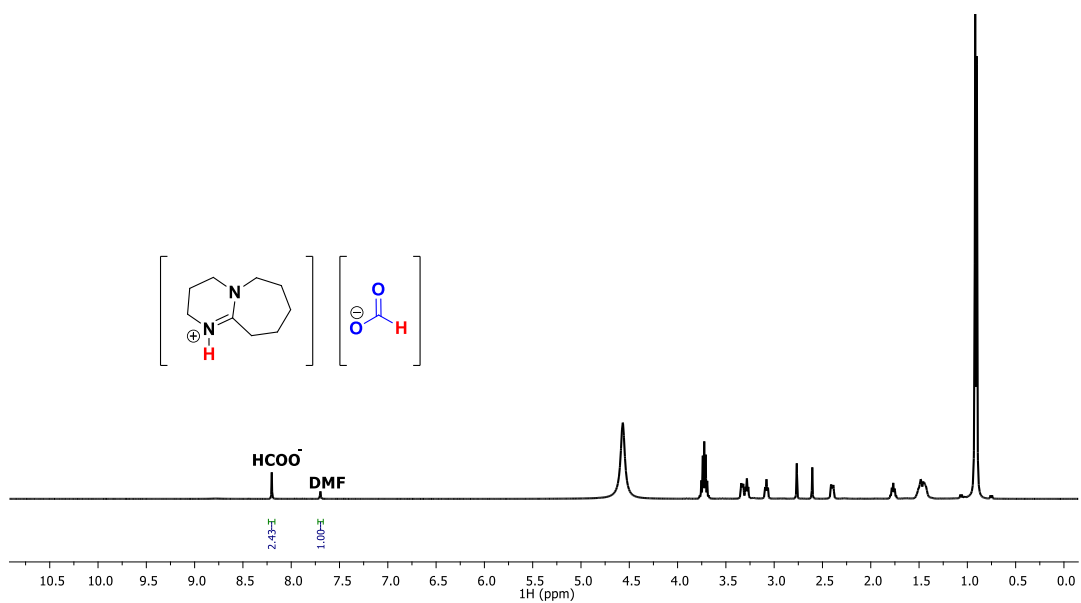


Figure S36. Conditions: **4**/DBU = 1/2000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 2).

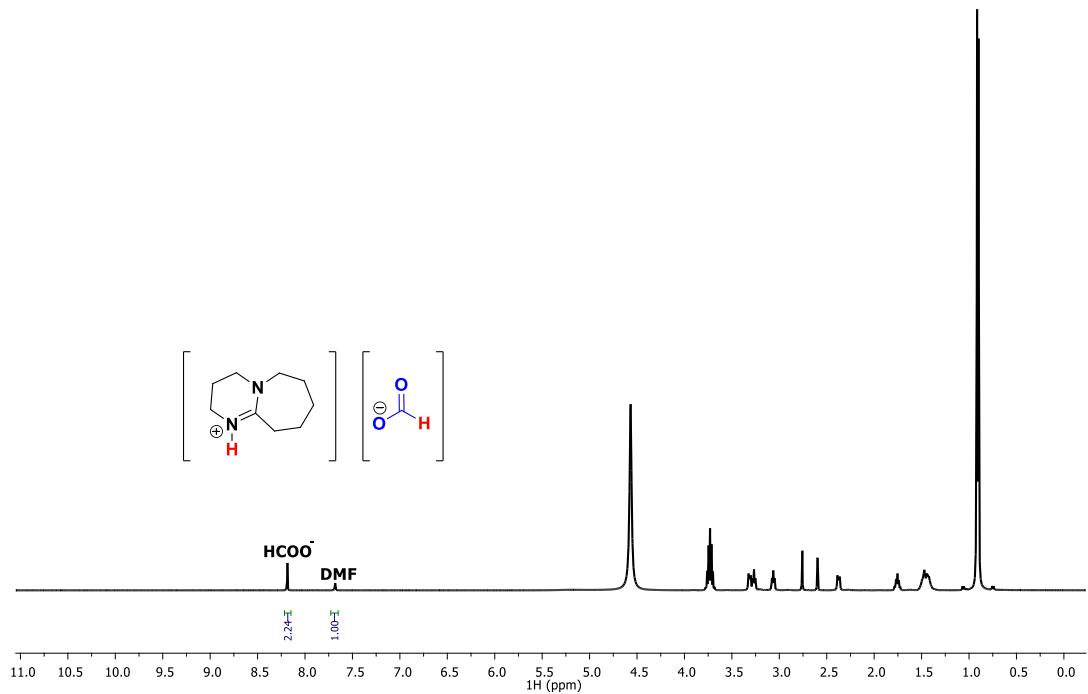


Figure S37. Conditions: **4**/DBU = 1/2000, **4**/LiOTf = 1/200, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 3).

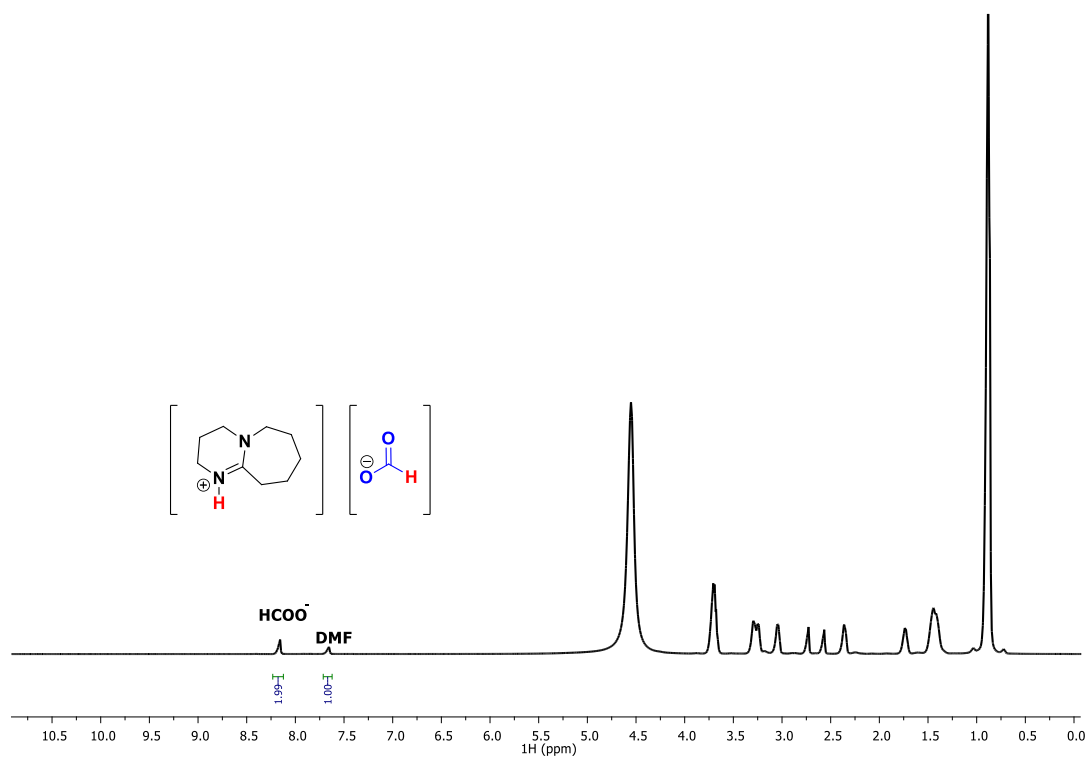


Figure S38. Conditions: **4**/DBU = 1/5000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 4).

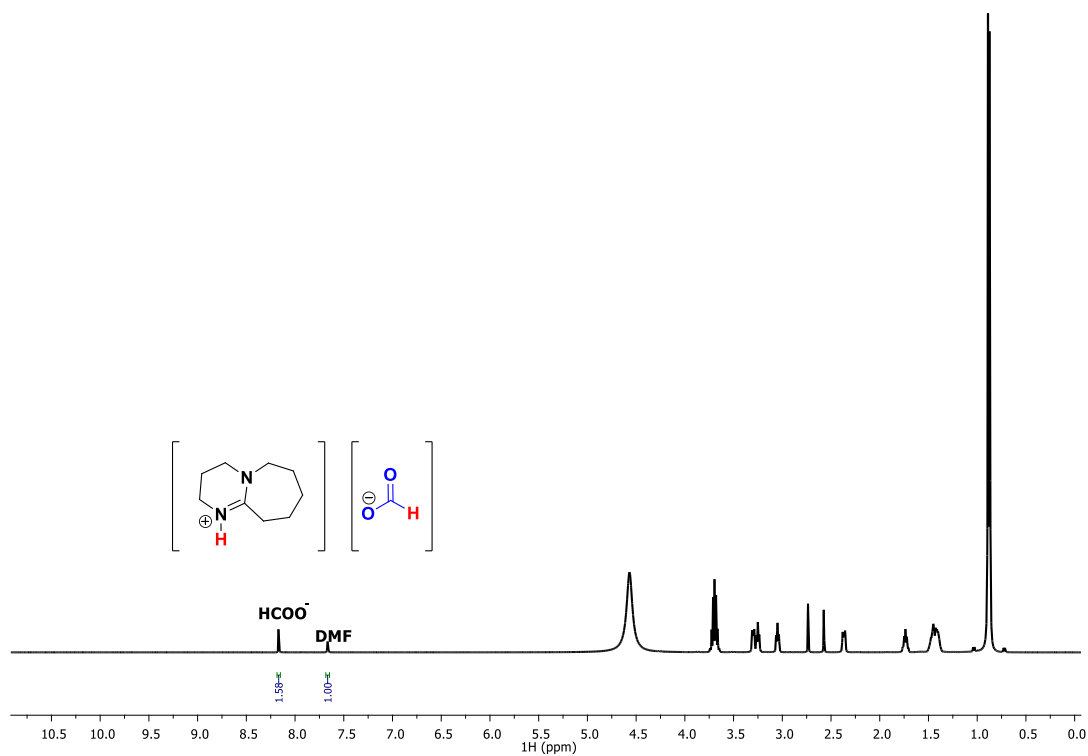


Figure S39. Conditions: **4**/DBU = 1/5000, **4**/LiOTf = 1/500, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 5).

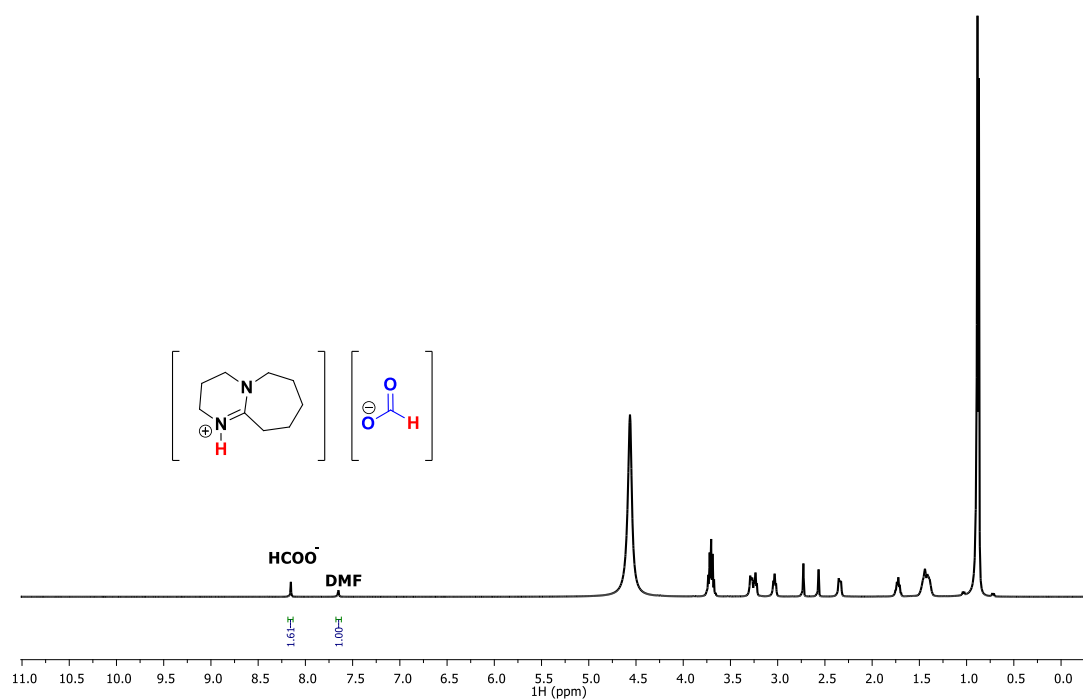


Figure S40. Conditions: **4**/DBU = 1/5000, **4**/LiOTf = 1/250, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 6).

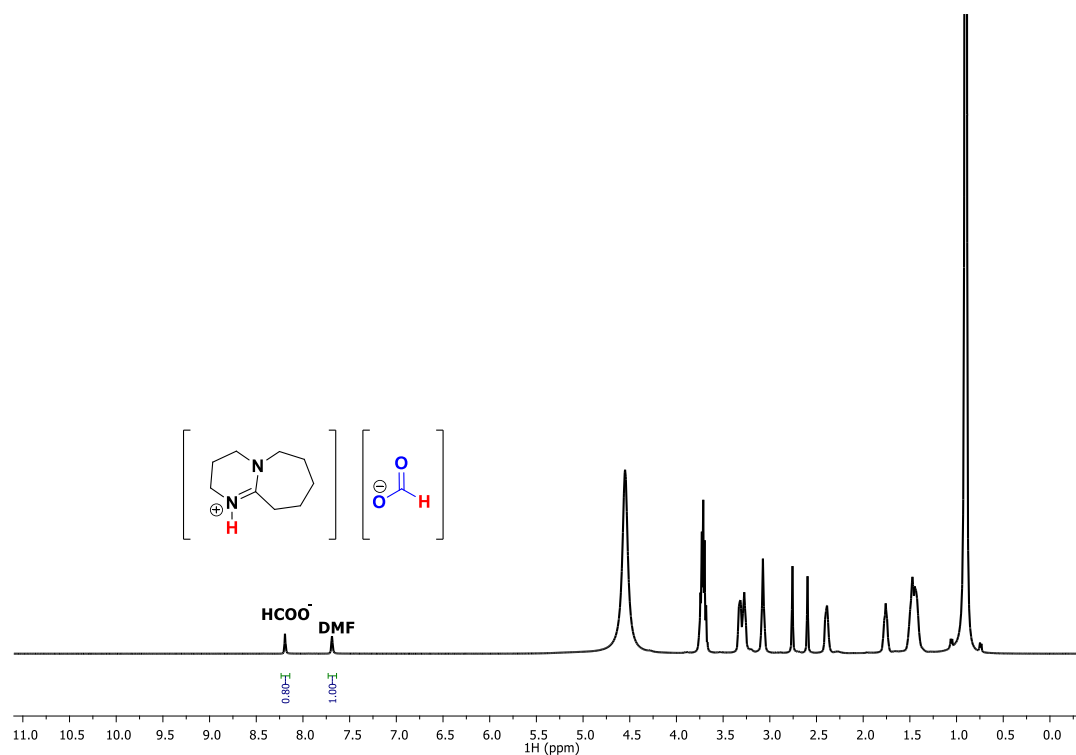


Figure S41. Conditions: **4**/DBU = 1/10 000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 7).

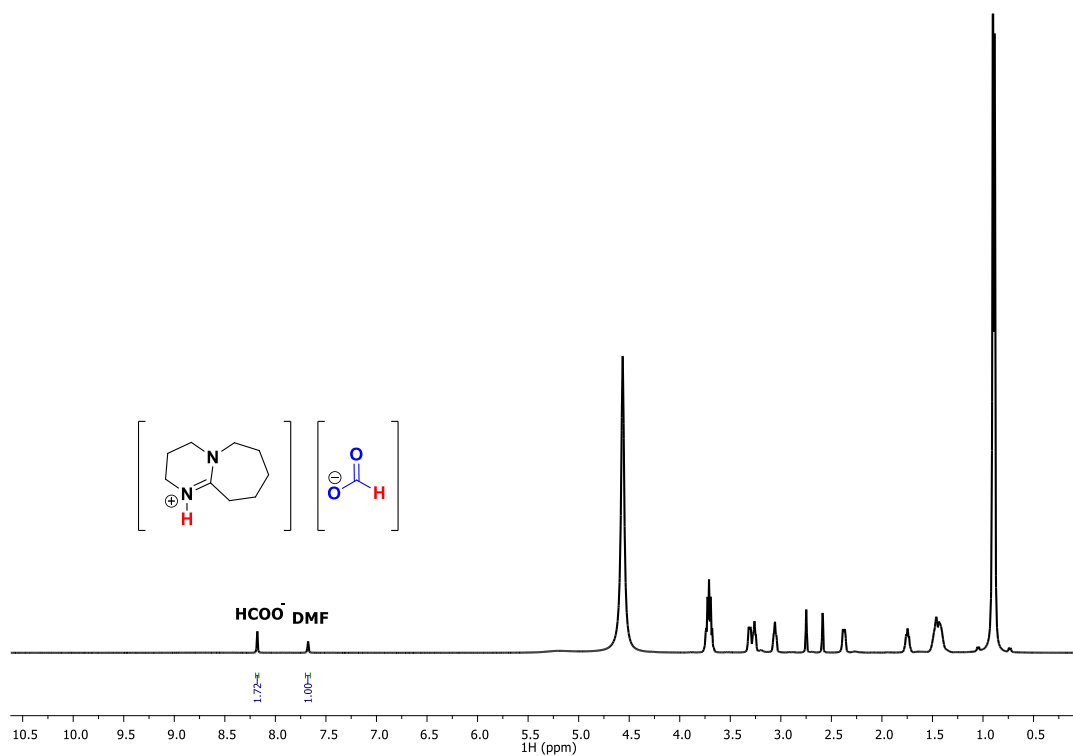


Figure S42. Conditions: **6**/DBU = 1/1000, ¹PrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 8).

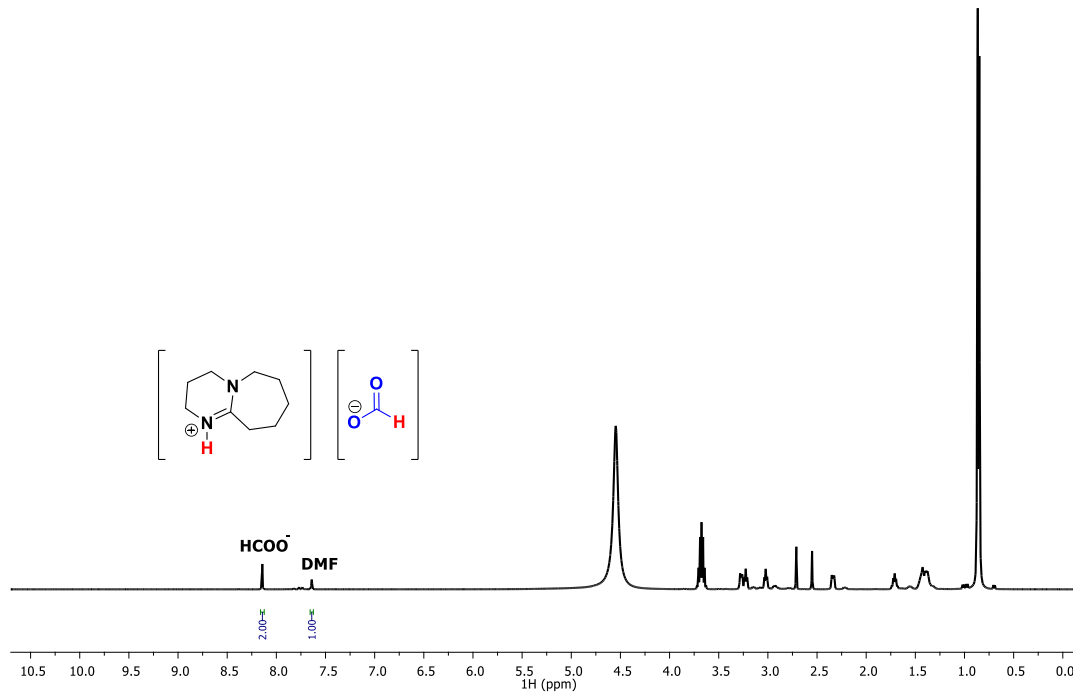


Figure S43. Conditions: **6**/DBU = 1/1000, ¹PrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 48 h (Entry 9).

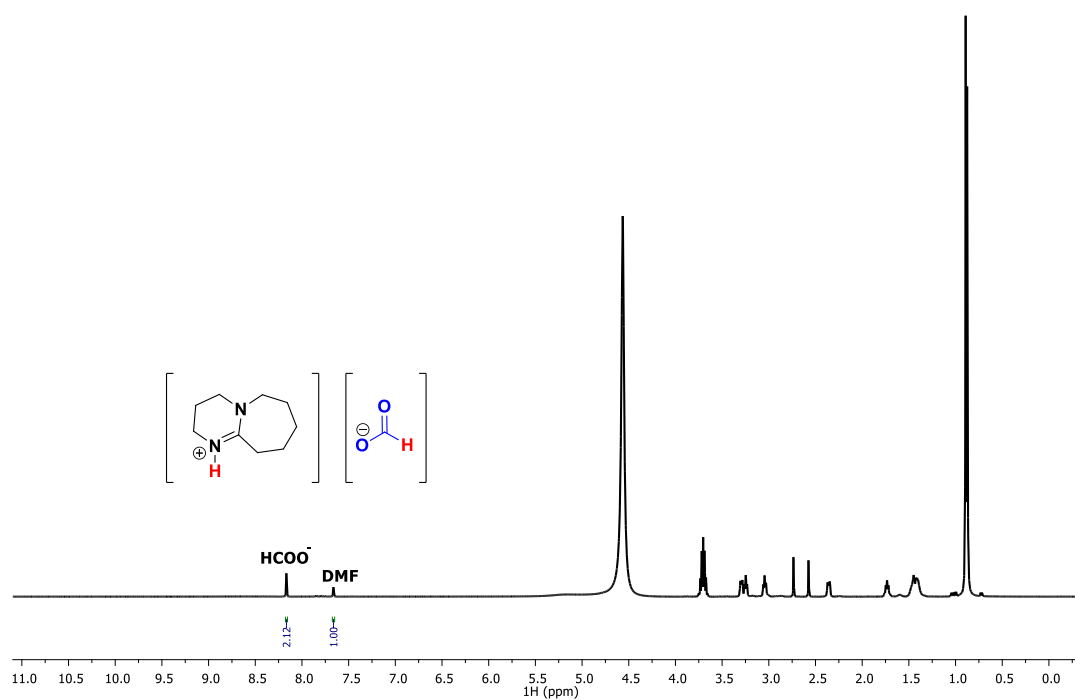


Figure S44. Conditions: **6**/DBU = 1/1000, **6**/LiOTf = 1/100, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 48 h (Entry 10).

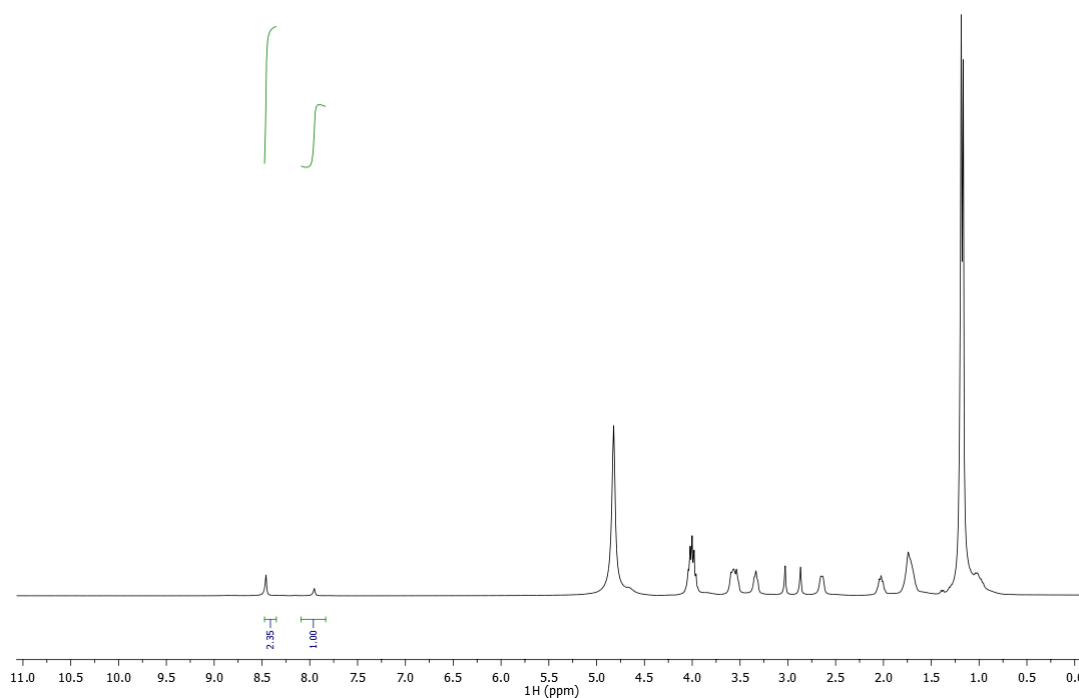


Figure S45. Conditions: **7**/DBU = 1/1000, **7**/LiOTf = 1/100, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 11).

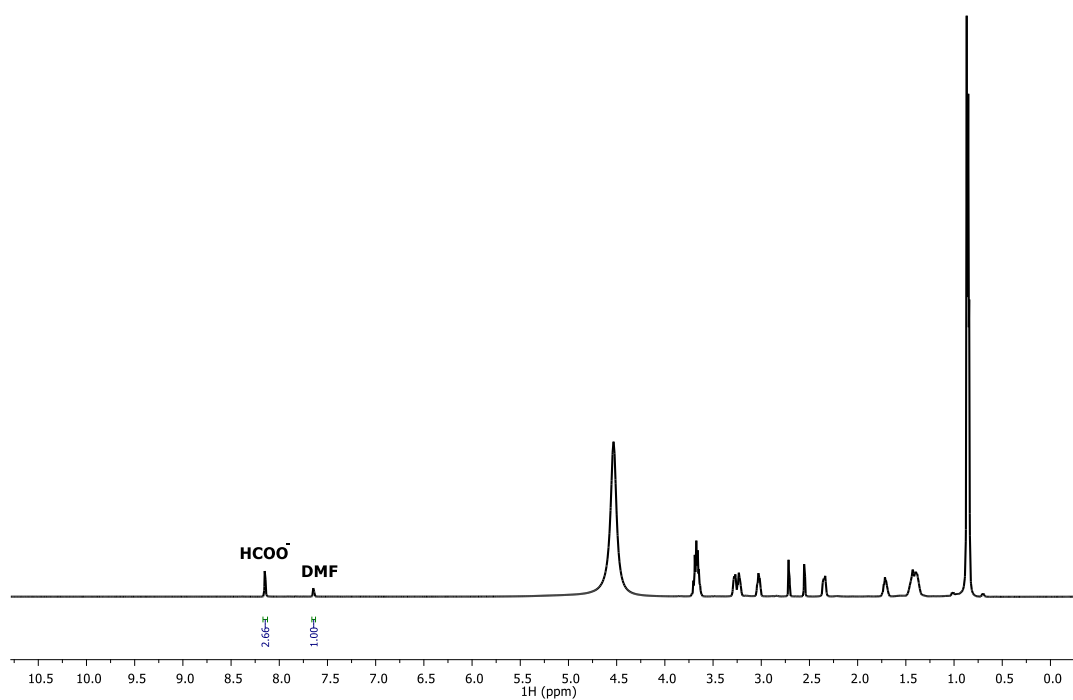


Figure S46. Conditions: **1**/DBU = 1/1000, ¹PrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 12).

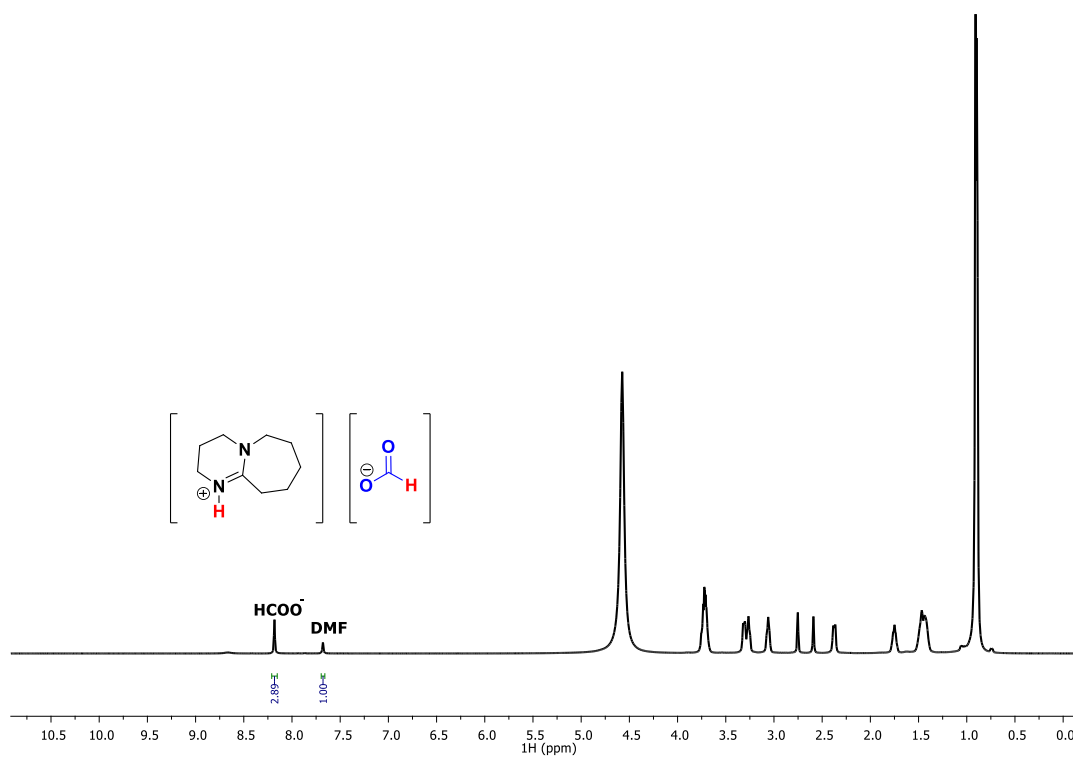


Figure S47. Conditions: **1**/DBU = 1/2000, ¹PrOH, pH₂/pCO₂ (bar) = 30/30, 100 °C, 24 h (Entry 13).

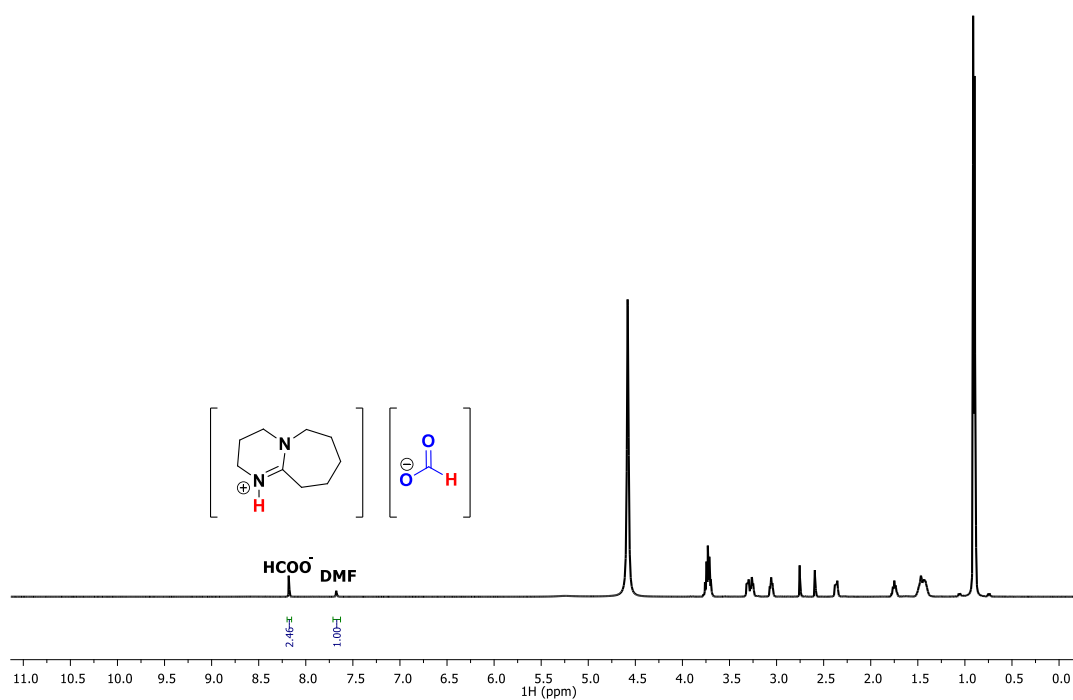


Figure S48. Conditions: **1**/DBU = 1/5000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 14).

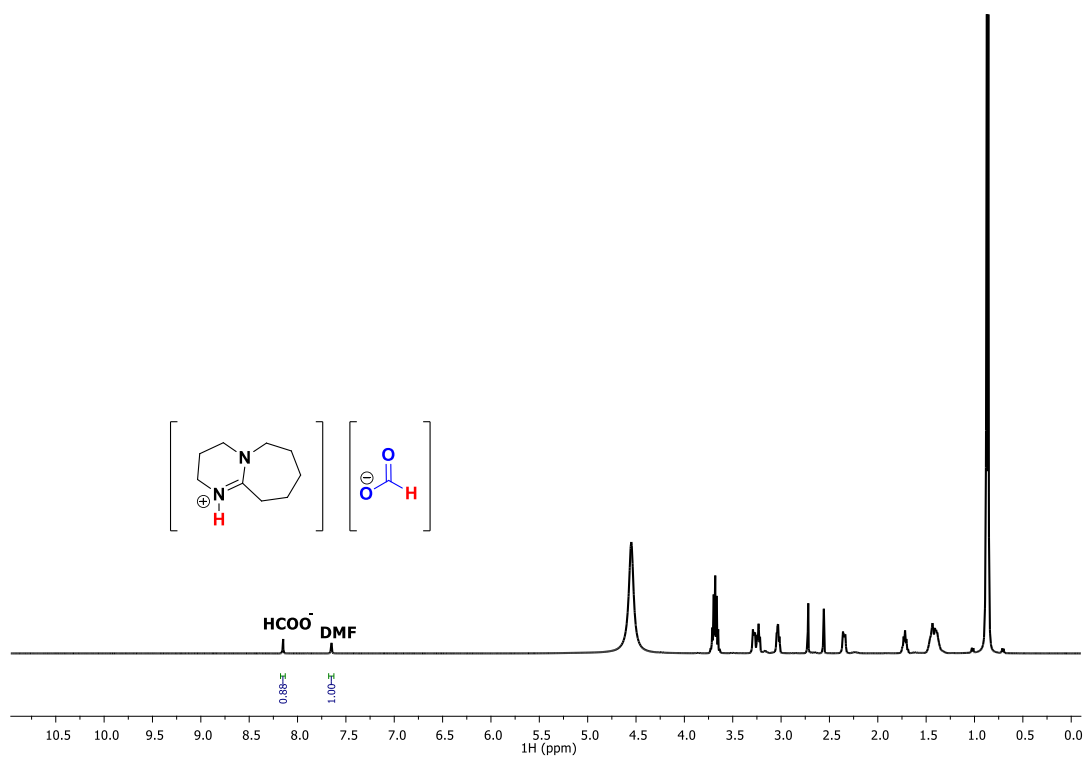


Figure S49. Conditions: **1**/DBU = 1/10 000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 15).

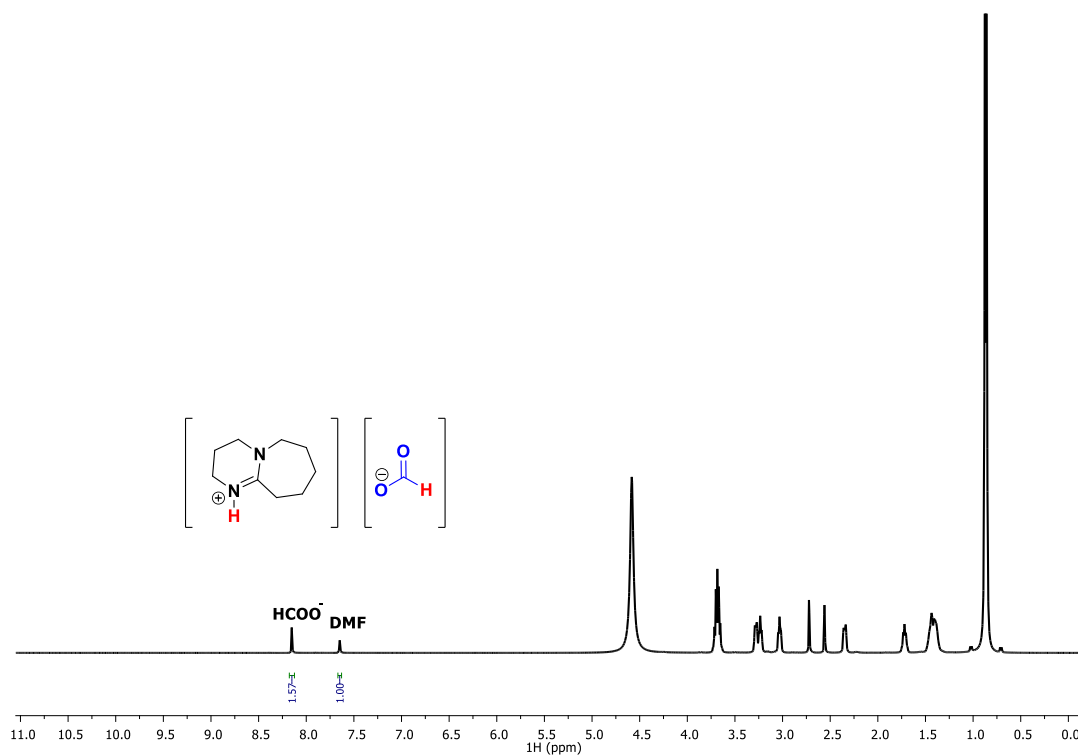


Figure S50. Conditions: **1**/DBU = 1/10 000, **1**/LiOTf = 1/1000, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 16).

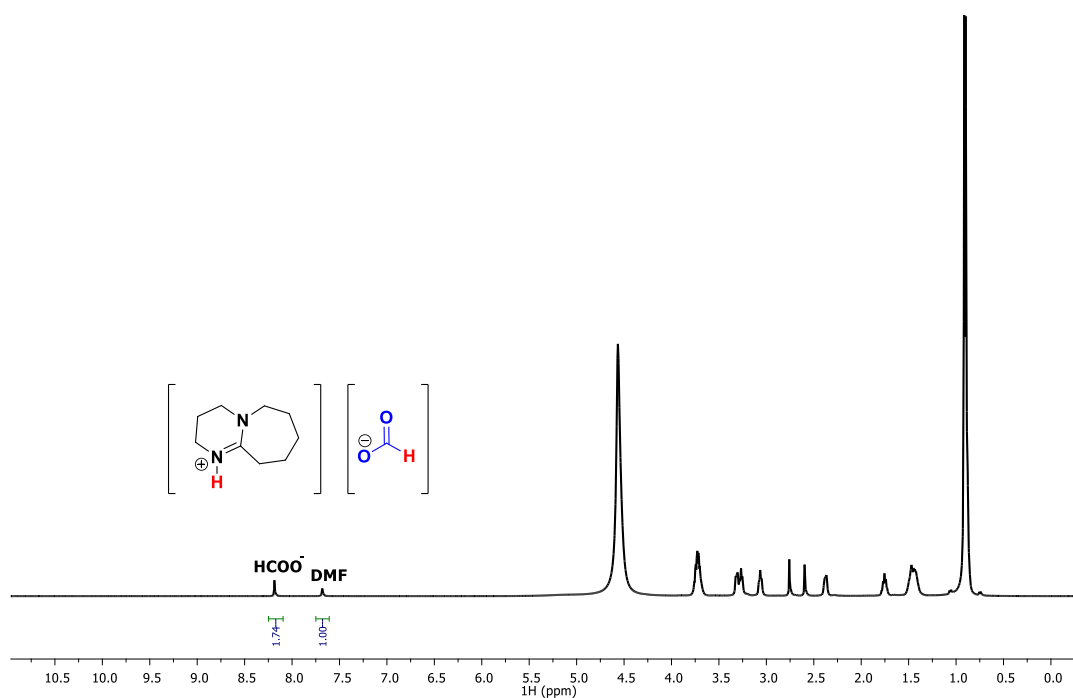


Figure S51. Conditions: **1**/DBU = 1/10 000, **1**/LiOTf = 1/500, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 17).

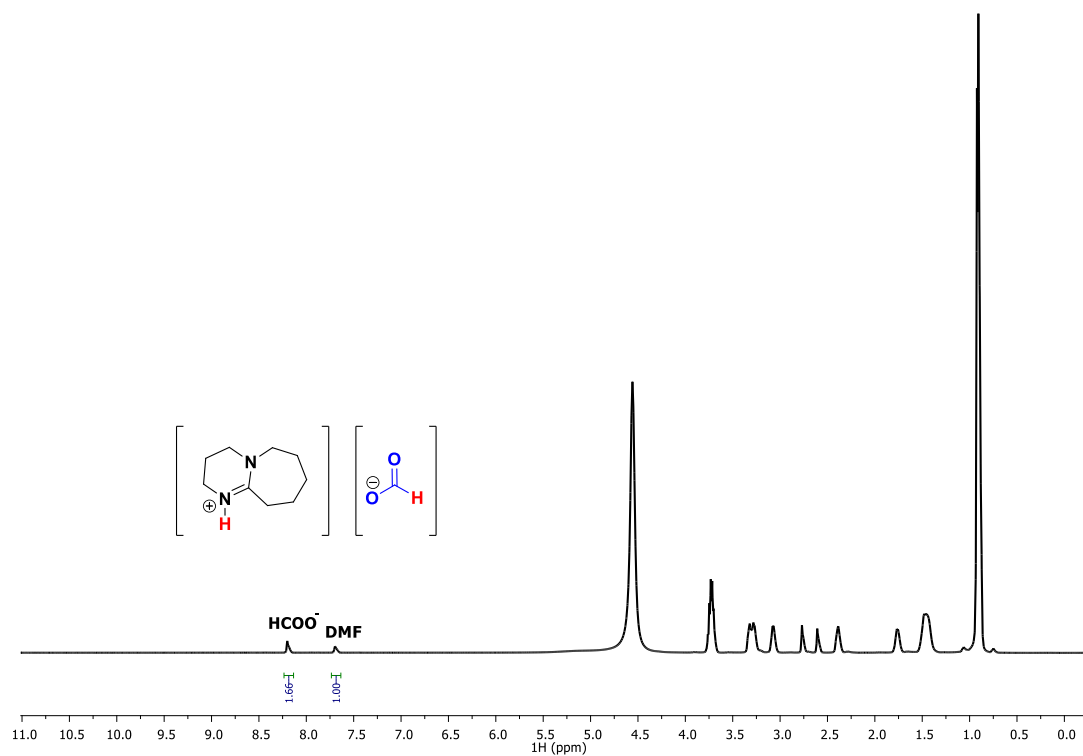


Figure S52. Conditions: **1**/DBU = 1/10 000, **1**/LiOTf = 1/250, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 18).

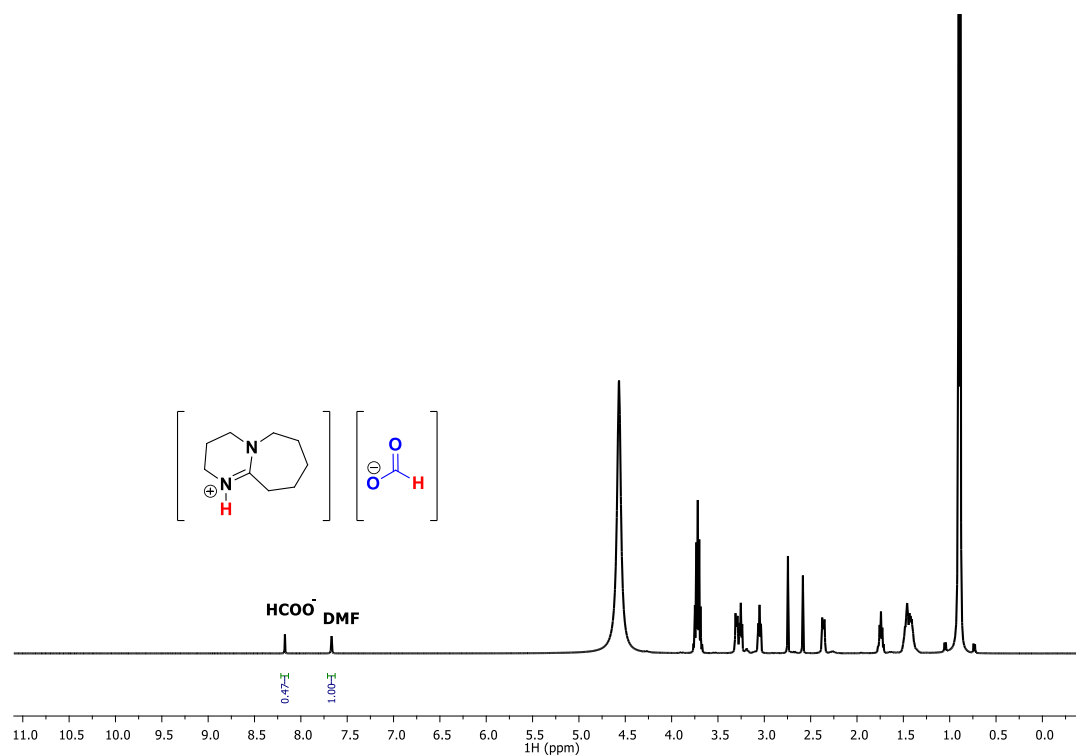


Figure S53. Conditions: **1**/DBU = 1/20 000, **1**/LiOTf = 1/500, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 100 °C, 24 h (Entry 19).

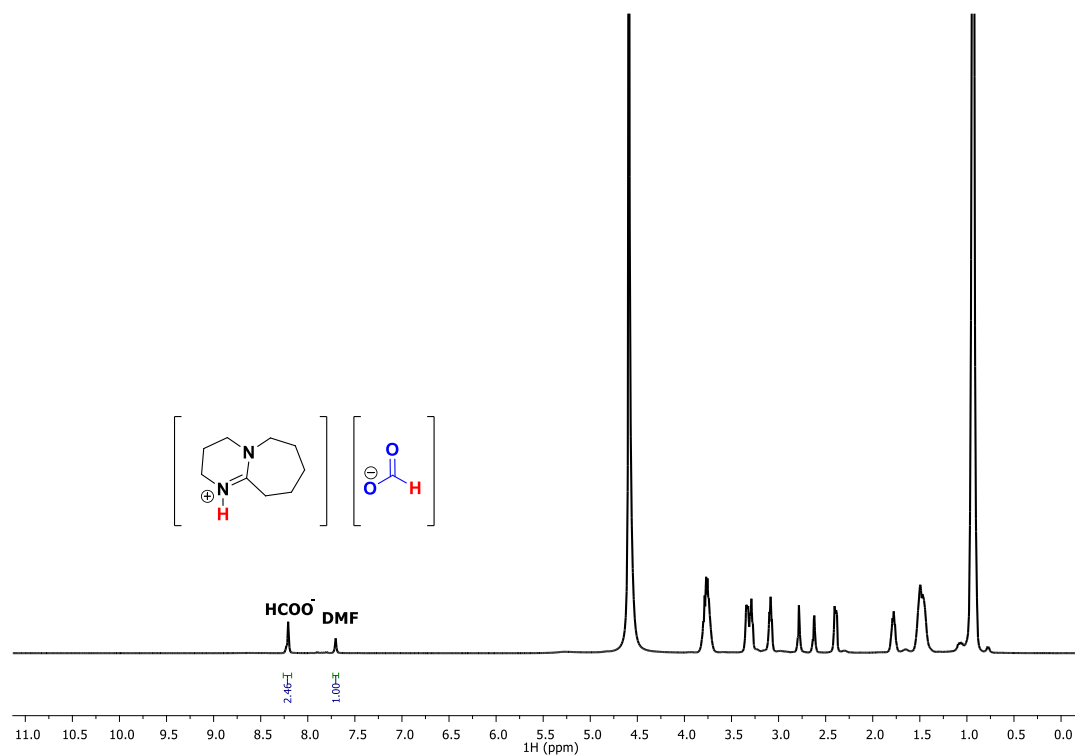


Figure S54. Conditions: **1**/DBU = 1/10 000, **1**/LiOTf = 1/250, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 120 °C, 24 h (Entry 20).

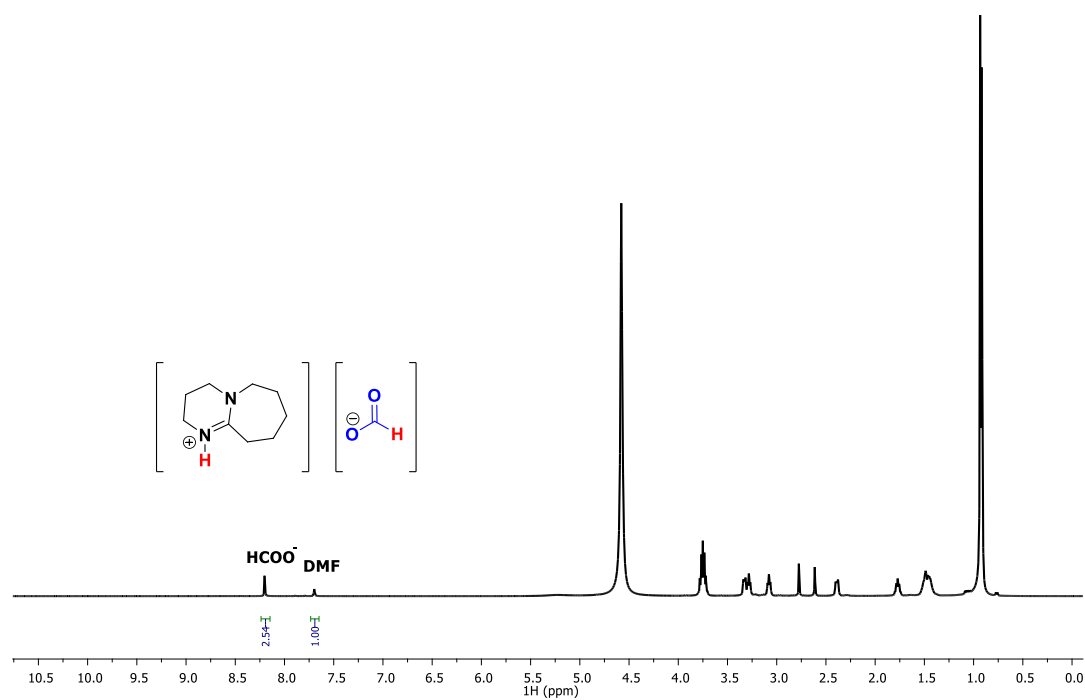


Figure S55. Conditions: **1**/DBU = 1/20 000, **1**/LiOTf = 1/500, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 120 °C, 24 h (Entry 21).

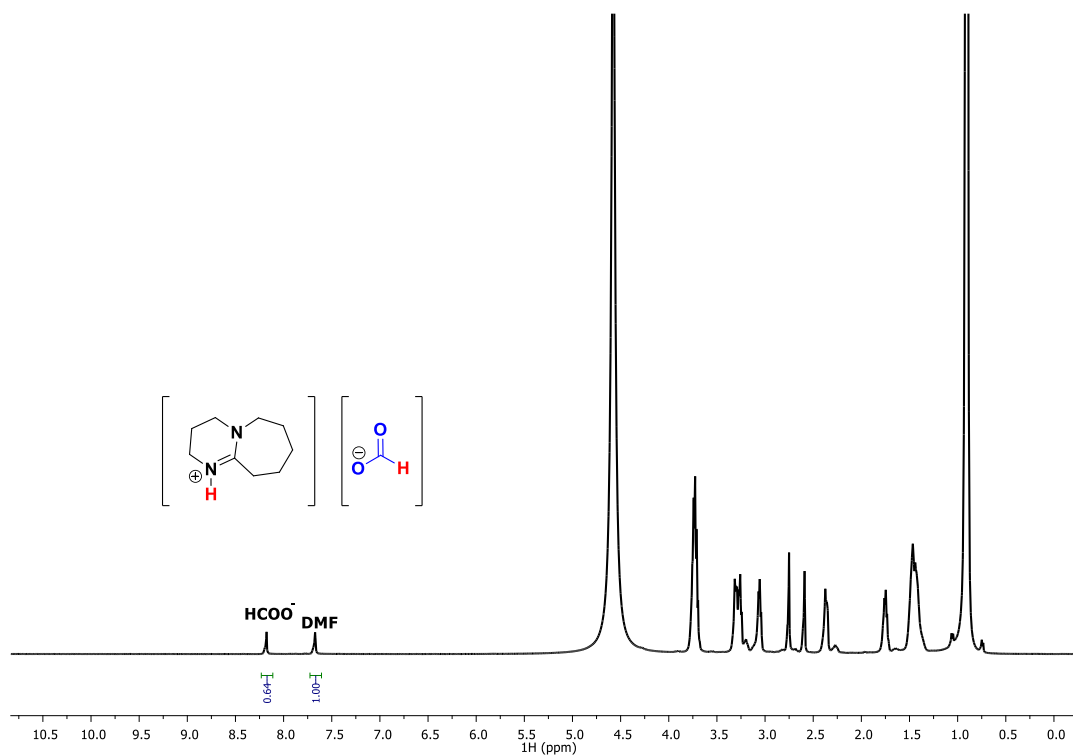


Figure S56. Conditions: **1**/DBU = 1/50 000, **1**/LiOTf = 1/1250, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 30/30, 120 °C, 24 h (Entry 22).

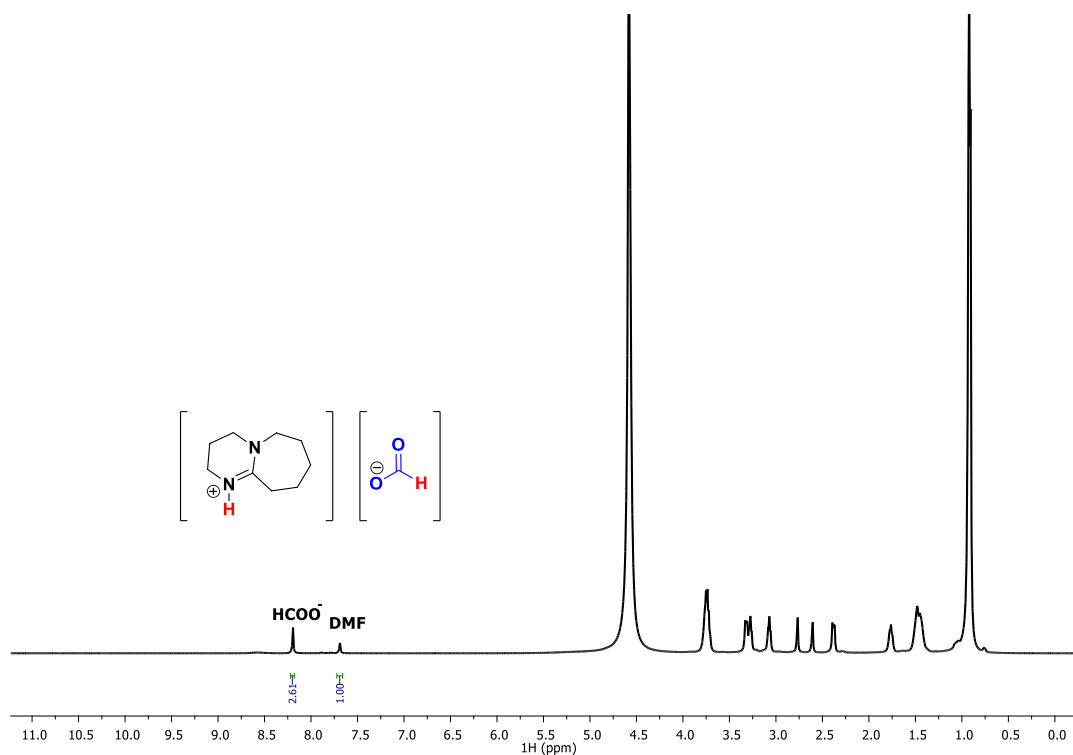


Figure S57. Conditions: **1**/DBU = 1/20 000, **1**/LiOTf = 1/500, ⁱPrOH, p_{H₂}/p_{CO₂} (bar) = 40/40, 120 °C, 24 h (Entry 23).

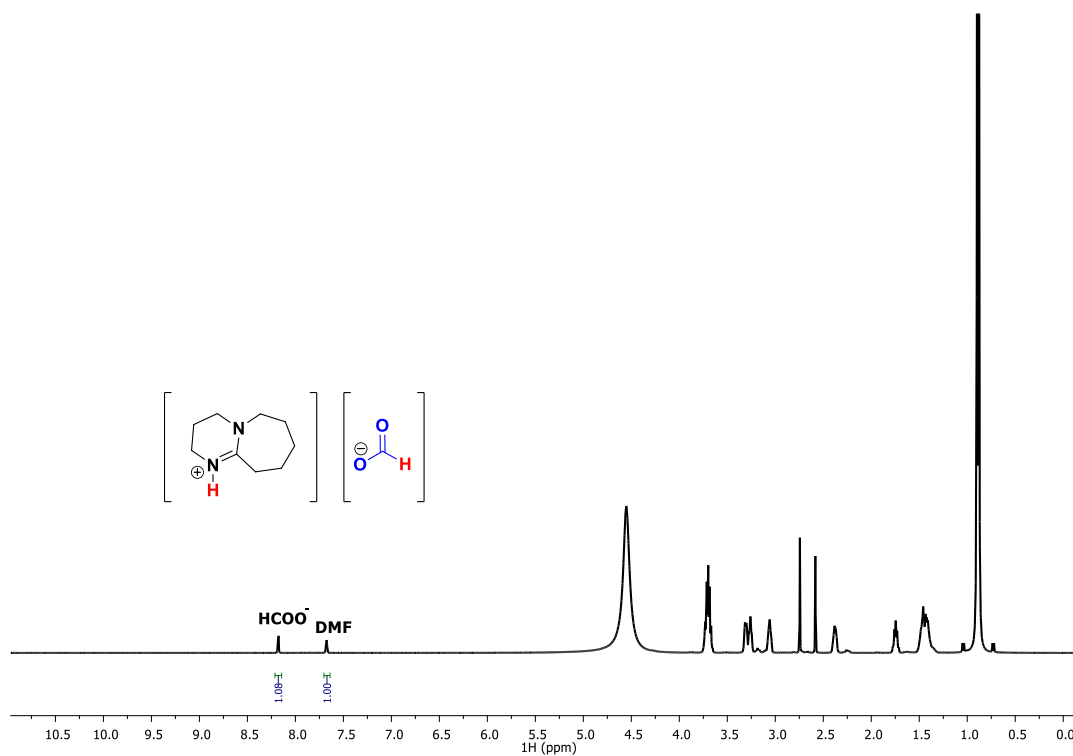


Figure S58. Conditions: **1**/DBU = 1/50 000, **1**/LiOTf = 1/1250, ⁱPrOH, pH₂/pCO₂ (bar) = 40/40, 120 °C, 24 h (Entry 25).

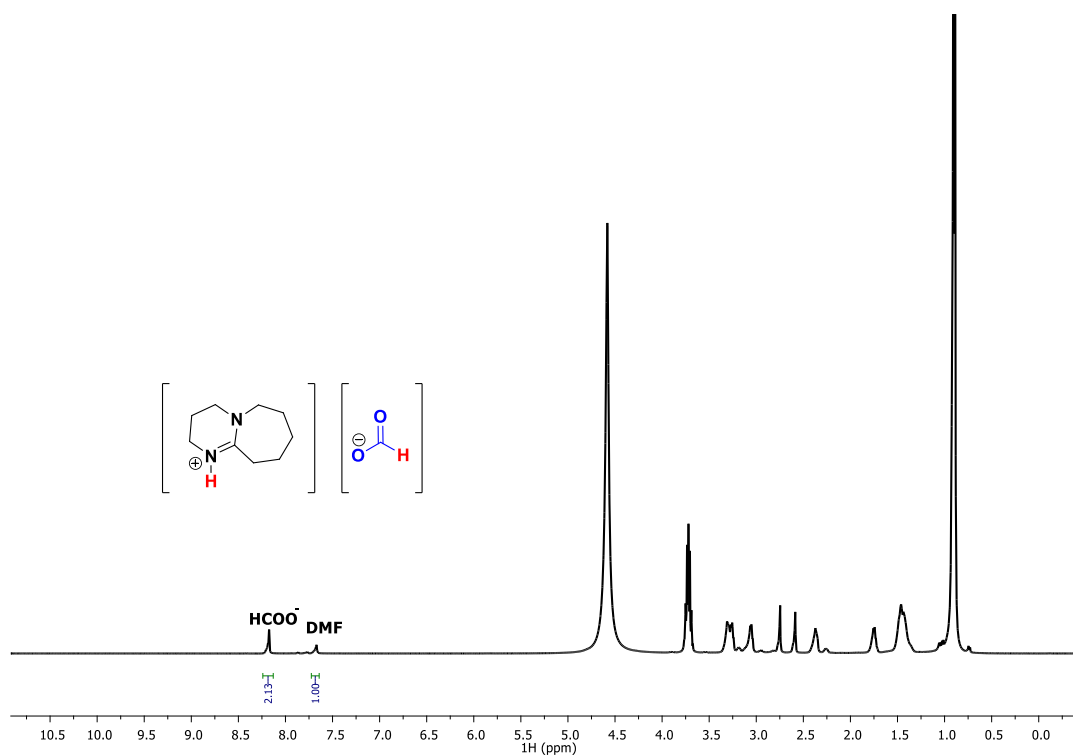


Figure S59. Conditions: **1**/DBU = 1/50 000, **1**/LiOTf = 1/1250, ⁱPrOH, pH₂/pCO₂ (bar) = 40/40, 120 °C, 48 h (Entry 26).

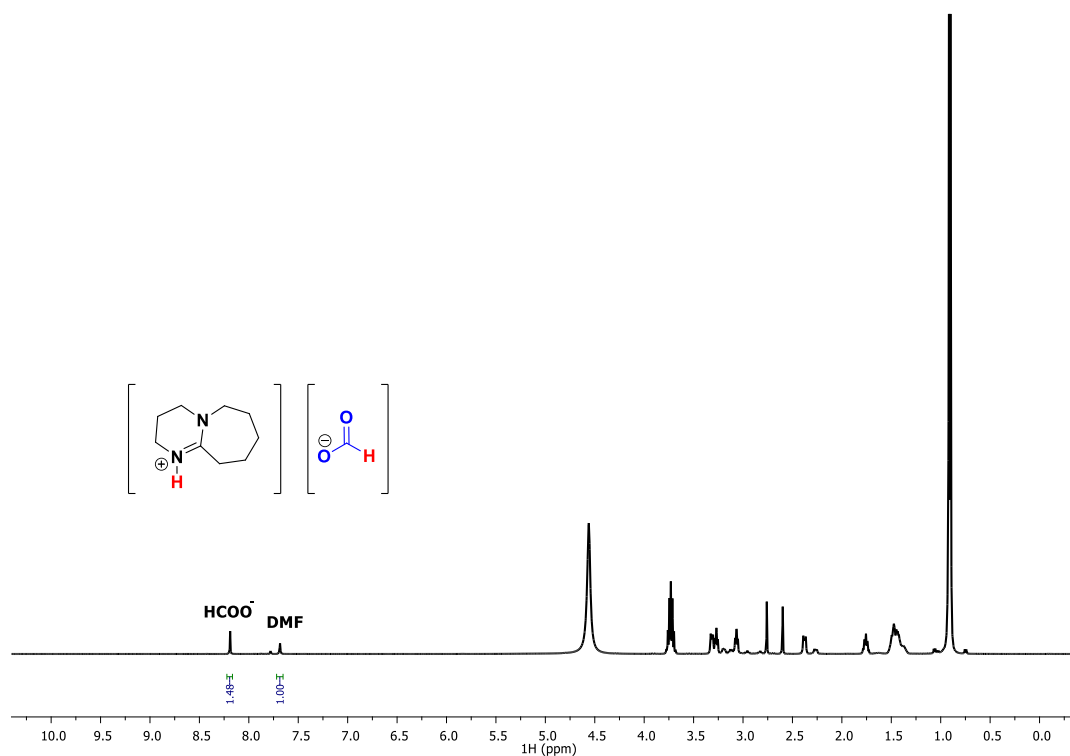


Figure S60. Conditions: **1**/DBU = 1/100 000, **1**/LiOTf = 1/2500, *i*PrOH, p_{H_2}/p_{CO_2} (bar) = 40/40, 120 °C, 96 h (Entry 27).

4. NMR Spectra of Mechanistic Experiments

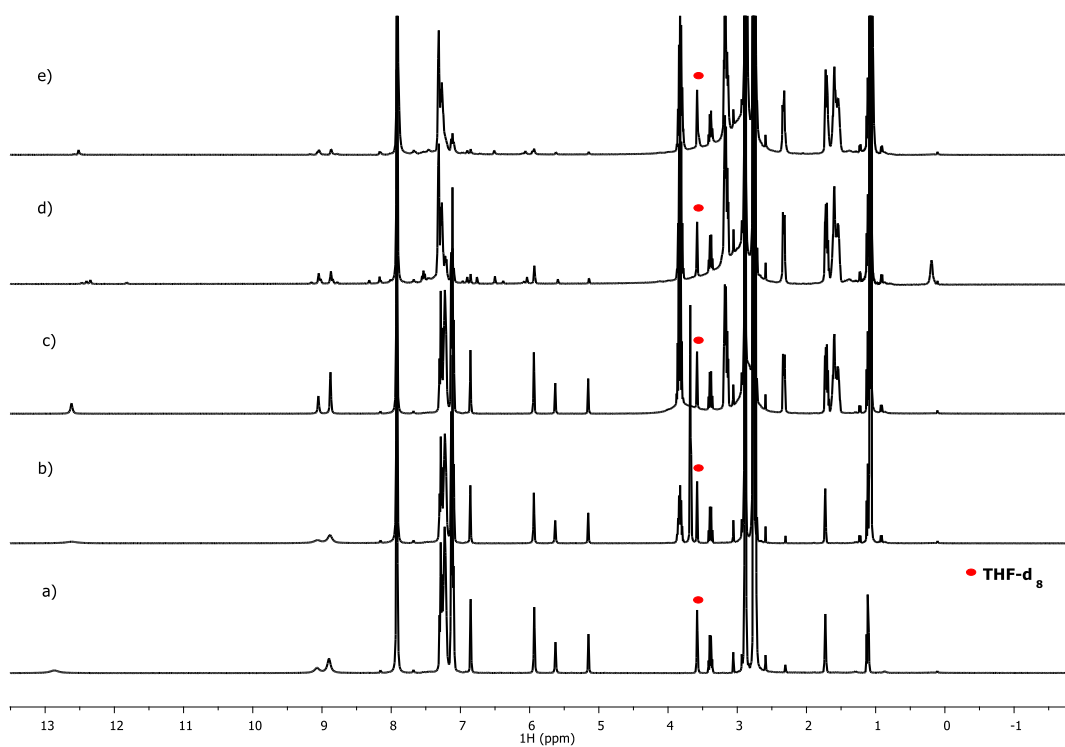


Figure S61. 1H NMR (THF- d_8). a) Complex **4**; b) *i*PrOH (10 equiv. to **4**); c) DBU (5 equiv. to **4**); d) after 1 h at 60 °C; e) after 24 h at 60 °C.

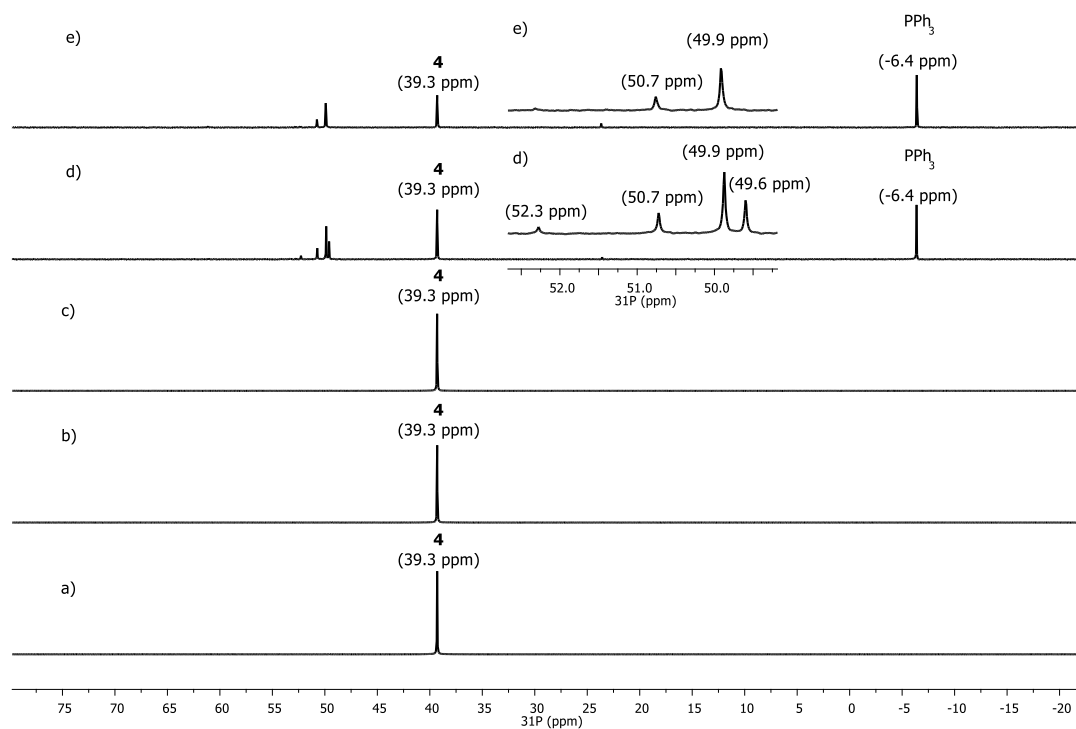


Figure S62. $^{31}\text{P}\{^1\text{H}\}$ NMR ($\text{THF-}d_8$). a) Complex **4**; b) $i\text{PrOH}$ (10 equiv. to **4**); c) DBU (5 equiv. to **4**); d) after 1 h at 60 °C; e) after 24 h at 60 °C.

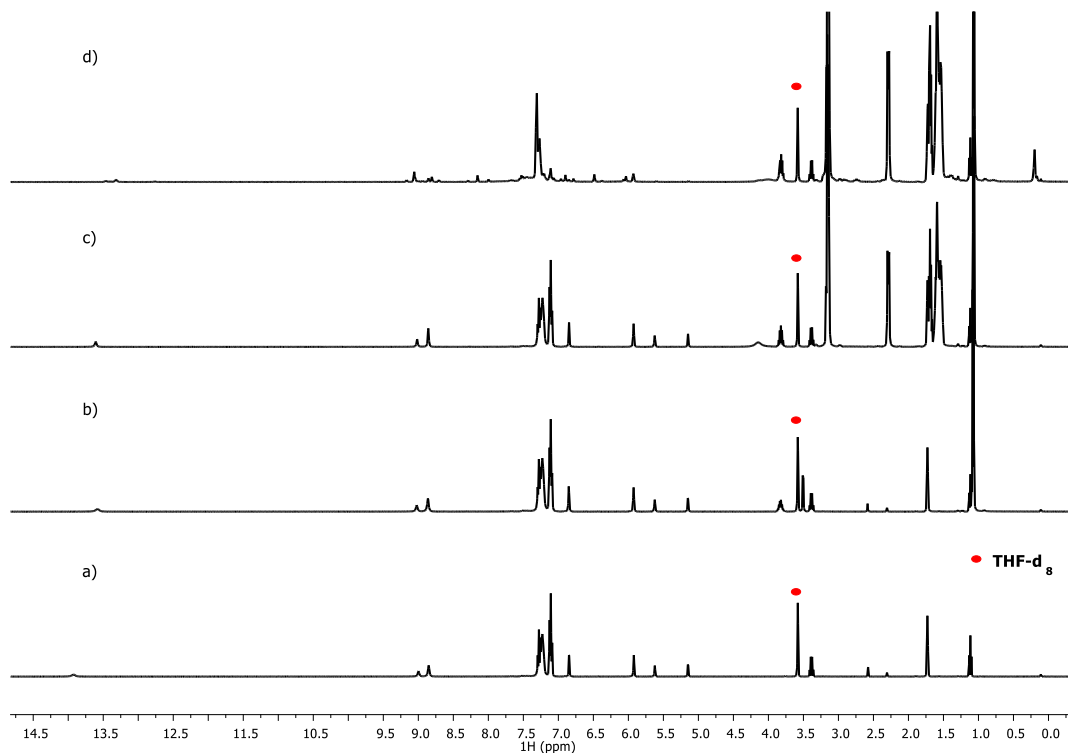


Figure S63. ^1H NMR ($\text{THF-}d_8$). a) Complex **4**; b) $i\text{PrOH}$ (2 equiv. to **4**); c) DBU (2 equiv. to **4**); d) after 1 h at 60 °C.

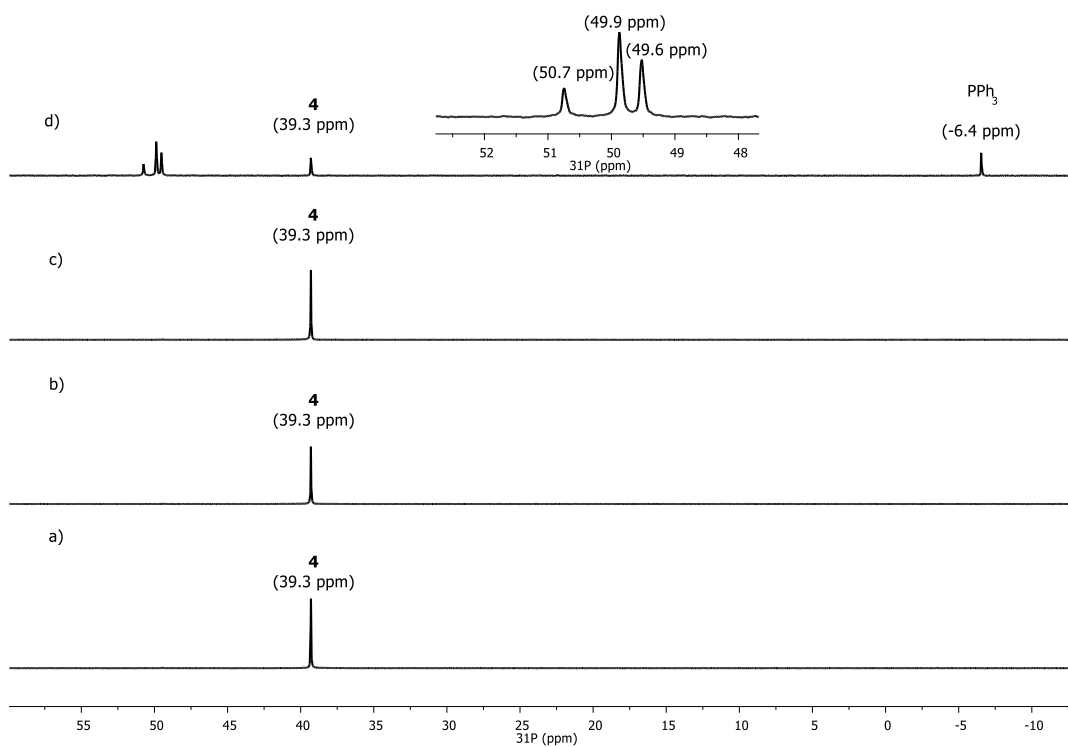


Figure S64. $^{31}\text{P}\{^1\text{H}\}$ NMR ($\text{THF-}d_8$). a) Complex 4; b) $i\text{PrOH}$ (2 equiv. to 4); c) DBU (2 equiv. to 4); d) after 1 h at 60 °C.

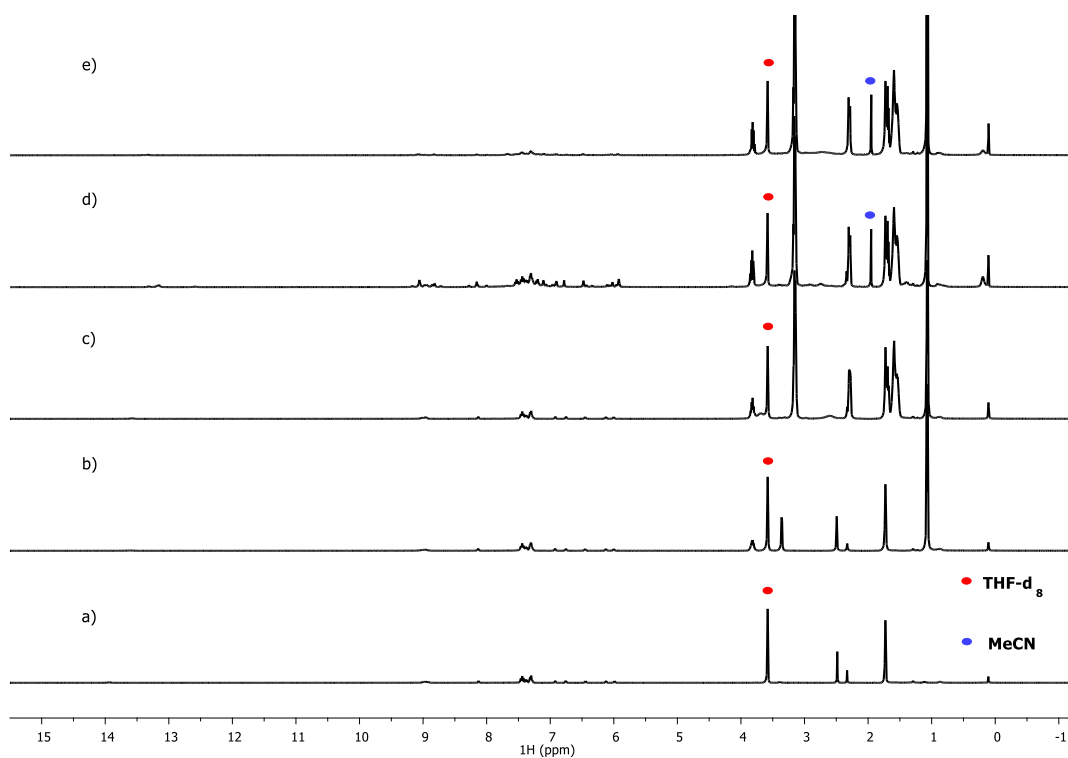


Figure S65. ^1H NMR ($\text{THF-}d_8$). a) Complex 1; b) $i\text{PrOH}$ (2 equiv. to 1); c) DBU (2 equiv. to 1); d) after 1 h at 60 °C; e) after 24 h at 60 °C.

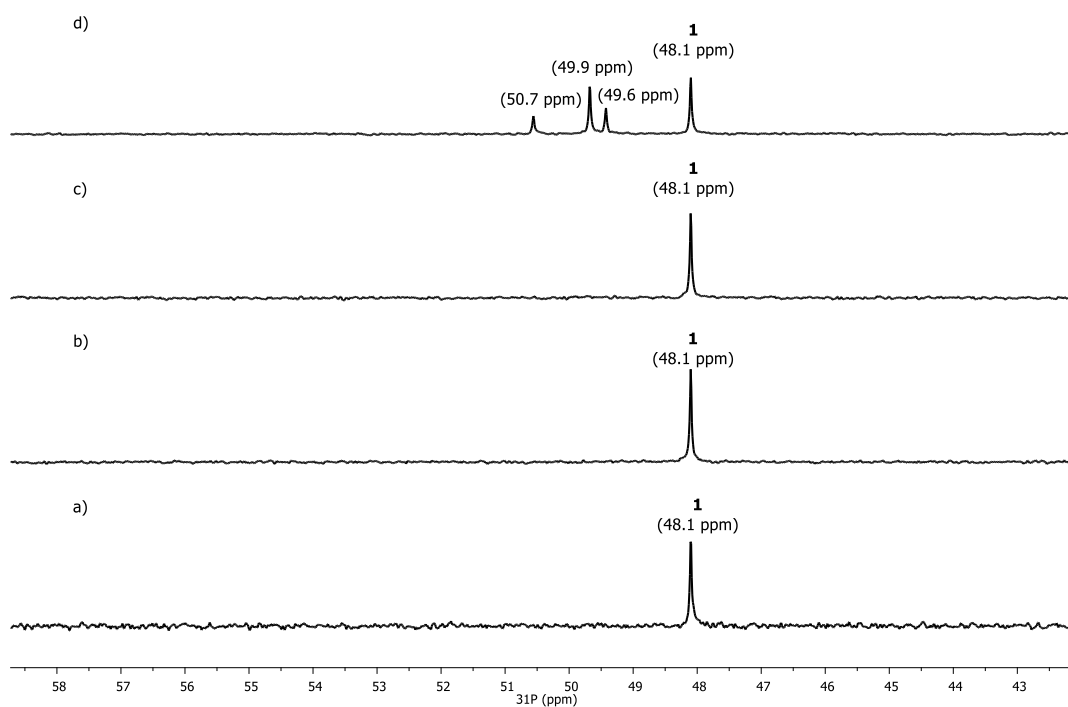


Figure S66. ^{31}P NMR ($\text{THF-}d_8$). a) Complex **1**; b) $i\text{PrOH}$ (2 equiv. to **1**); c) DBU (2 equiv. to **1**); d) after 1 h at 60 $^{\circ}\text{C}$.

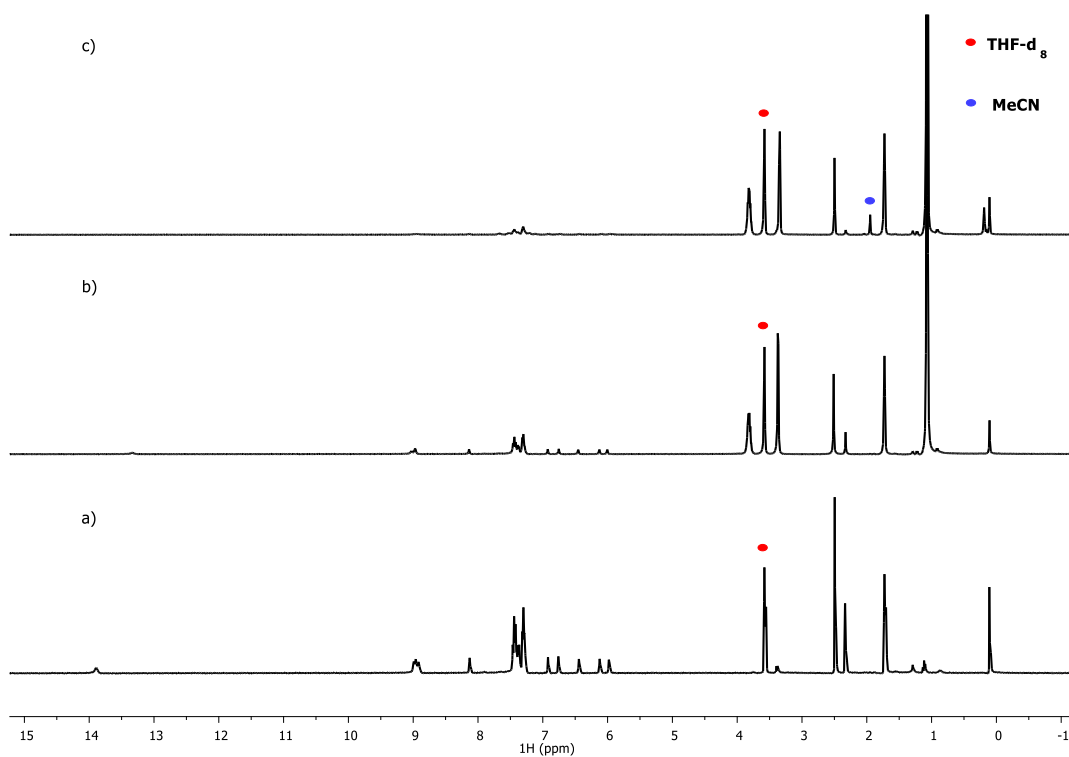


Figure S67. ^1H NMR ($\text{THF-}d_8$). a) Complex **1**; b) $i\text{PrOH}$ (2 equiv. to **1**); c) after 15 min at 60 $^{\circ}\text{C}$.

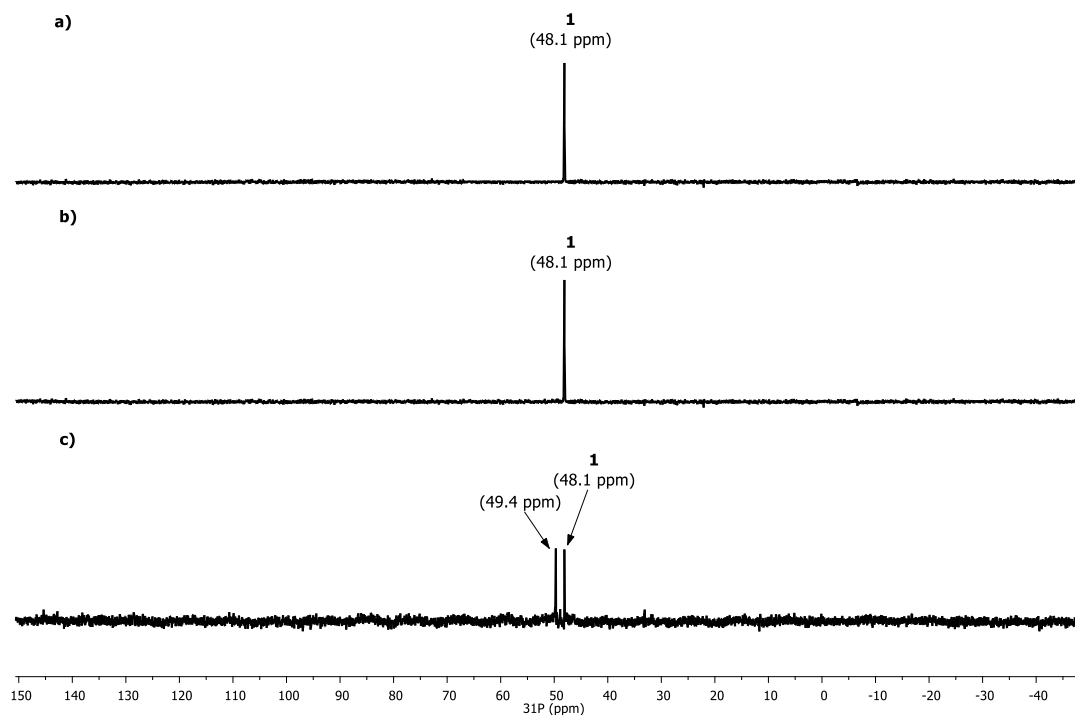


Figure S68. $^{31}\text{P}\{^1\text{H}\}$ NMR, ($\text{THF-}d_8$). a) Complex **1**; b) $i\text{PrOH}$ (2 equiv. to **1**) c) after 15 min at 60 °C.

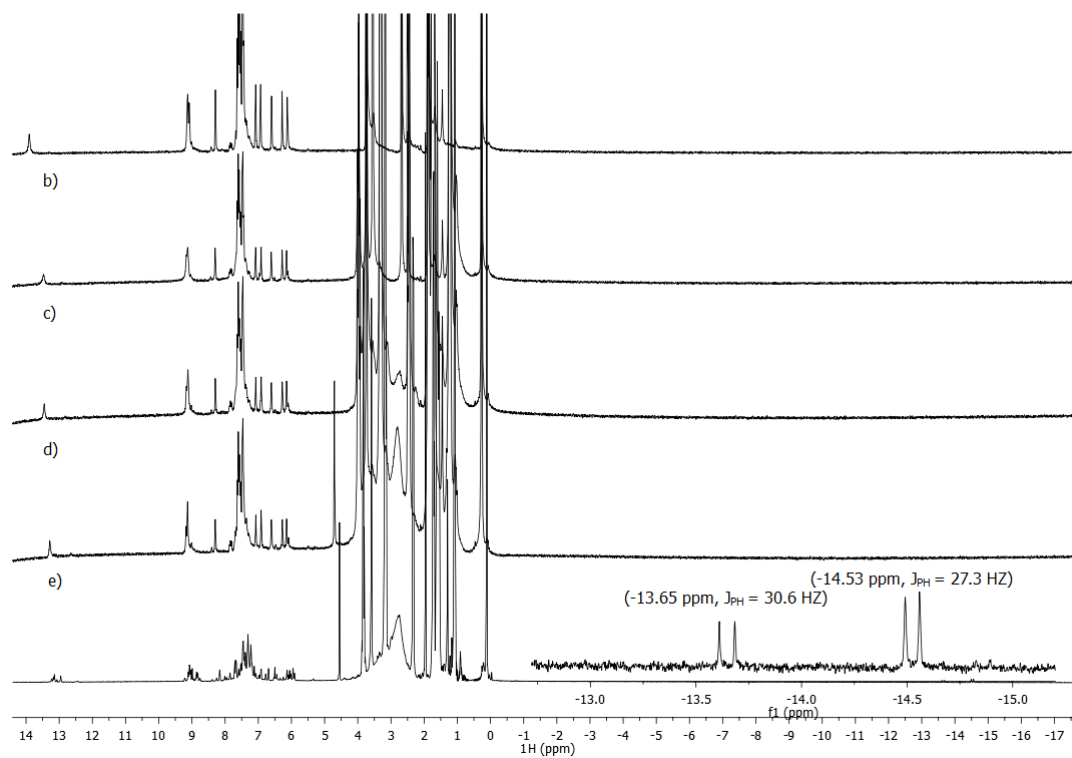


Figure S69. ^1H NMR, ($\text{THF-}d_8$). a) Complex **1**; b) after addition of $i\text{PrOH}$ (2 equiv.) c) after addition of DBU (2 equiv.); d) after addition of H_2 gas (1 bar); e) after heating to 60 °C for 12 h.

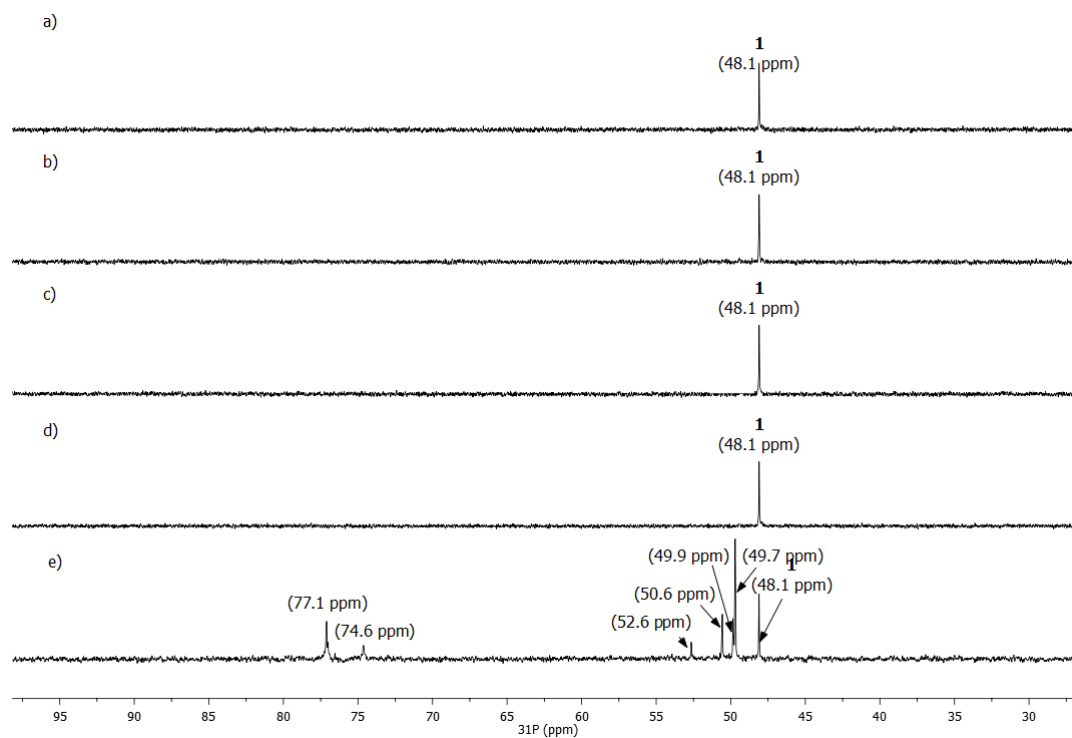


Figure S70. $^{31}\text{P}\{^1\text{H}\}$ NMR, ($\text{THF-}d_8$). a) Complex **1**; b) after addition of $i\text{PrOH}$ (2 equiv.) c) after addition of DBU (2 equiv.); d) after addition of H_2 gas (1 bar); e) after heating to 60°C for 12 h.

5. X-ray Crystallographic Tables

Crystal data and collection details for complexes **8·H₂O**, **9·solv** and **10·solv** are reported in Table S1. Data for **8·H₂O** and **9·solv** were recorded on a Bruker APEX II diffractometer equipped with a PHOTON2 detector using Mo–K α radiation. Data for **10·solv** were recorded on a Bruker D8 Venture equipped with a microfocus Mo source (K α radiation) and a 2D Photon III detector. Data were corrected for Lorentz polarization and absorption effects (empirical absorption correction SADABS) [5]. The structures were solved by direct methods [6] and refined by full-matrix least-squares based on all data using F^2 . Hydrogen atoms were fixed at calculated positions and refined by a riding model. All non-hydrogen atoms were refined with anisotropic displacement parameters. The unit cells of **9·solv** and **10·solv** contain additional total potential solvent accessible voids of 507 Å³ and 245 Å³ (ca. 7 and 6 % of the Cell Volume, respectively), which are likely to be occupied by highly disordered solvent molecules. These voids were treated using the SQUEEZE routine of PLATON [7].

Table S1. Crystal data and measurement details for **8·H₂O**, **9·solv** and **10·solv**.

	8·H₂O	9·solv	10·solv
CCDC number	2413084	2413085	2413086
Formula	C ₃₀ H ₃₅ N ₁₀ O ₈ PRu	C ₃₄ H ₃₃ N ₁₀ O ₆ PRu	C ₄₀ H ₃₃ N ₁₀ O ₆ PRu
FW	795.72	809.74	881.80
T, K	100(2)	100(2)	100(2)
λ , Å	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$C2/c$	$P2_1/n$
<i>a</i> , Å	11.4034(8)	37.307(3)	14.7342(4)
<i>b</i> , Å	13.9105(10)	12.5534(9)	17.0807(4)
<i>c</i> , Å	21.7313(15)	15.7761(11)	16.1085(4)
α , °	90	90	90
β , °	98.356(2)	101.422(2)	97.4200(10)
γ , °	90	90	90
Cell Volume, Å ³	3410.6(4)	7242.1(9)	4020.08(18)
Z	4	8	4
D_c , g·cm ⁻³	1.550	1.485	1.457
μ , mm ⁻¹	0.571	0.536	0.490
F(000)	1632	3312	1800
Crystal size, mm	0.150×0.130×0.1 10	0.220×0.210×0.1 70	0.131×0.084×0.0 45
θ limits, °	1.744-25.198	1.715-25.050	2.007-29.127
Reflections collected	42804	39419	137081
Independent reflections	6141 [R_{int} = 0.0363]	6409 [R_{int} = 0.0610]	10808 [R_{int} = 0.0999]
Data / restraints / parameters	6141 / 395 / 514	6409 / 162 / 482	10808 / 0 / 554
Goodness on fit on F^2	1.282	1.331	1.049
R_1 ($I > 2\sigma(I)$)	0.0596	0.0900	0.0372
wR_2 (all data)	0.1481	0.2111	0.0845
Largest diff. peak and hole, e Å ⁻³	1.930 / -1.292	1.221 / -2.726	0.984 / -0.755

Table S2. Main bond distances (Å) and angles (°) for **8-10**.

	8	9	10
Ru1-N1	2.156(5)	2.123(6)	2.1137(18)
Ru1-N3	2.079(5)	2.091(7)	2.0825(18)
Ru1-N5	2.085(5)	2.082(7)	2.0750(18)
Ru1-N7	2.120(5)	2.056(7)	2.0679(18)
Ru1-N8	2.115(5)	2.109(6)	2.0588(18)
Ru1-P1	2.3008(14)	2.308(2)	2.3413(6)
N1-Ru1-N3	82.82(17)	84.3(3)	83.28(7)
N1-Ru1-N5	82.26(17)	84.0(3)	85.12(7)
N3-Ru1-N5	89.77(18)	86.4(3)	86.45(7)
N7-Ru1-N8	81.54(18)	80.0(3)	79.28(7)
N7-Ru1-P1	94.66(13)	96.79(19)	92.64(5)
N8-Ru1-P1	92.79(13)	95.89(19)	92.05(5)

The degree of distortion from the ideal geometry was evaluated using the δ parameter calculated using the Polynator software[8] and defined as:

$$\left(\frac{\sum_i |a_i - v_i|^2}{\sum_i |a_i - c|^2} \right)^{1/2}$$

where \mathbf{a}_i is an atom vector, \mathbf{v}_i is the vector of its corresponding model vertex and \mathbf{c} is the centroid of all atom vectors. A perfect match between a model and a set of vectors identified by the positions of the atoms directly coordinated to the metal gives δ value of 0. Table S3 lists the δ values for complexes **8**, **9** and **10**. The geometry of the central metal, in each of these four complexes can be classified as a distorted octahedron, since the δ values are significantly below 18 (the threshold beyond which the distortion is considered severe). The optimal geometry for **8-9** corresponds to a *tetragonal heterobipyramid* geometry, whereas a *parallelogrammic bipyramid* provides the best fit for **10**. In all cases, the greater longitudinal deviation along one of the four-fold symmetry axes from the ideal octahedron is attributed to the longer Ru–P bond length compared to the Ru–N bonds (see Table S2). This is illustrated in Figure S71.

Table S3. δ values of octahedron, tetragonal heterobipyramidal and parallelogrammic bipyramid shape models for complexes **8**, **9** and **10**.

	8	9	10
$\delta_{\text{octahedron [m-3m]}}$	7.872	8.914	8.567
$\delta_{\text{tetragonalheterobipyramid [4mm]}}$	5.654	5.970	7.792
$\delta_{\text{parallelogrammicbipyramid [2/m]}}$	6.708	7.010	6.083

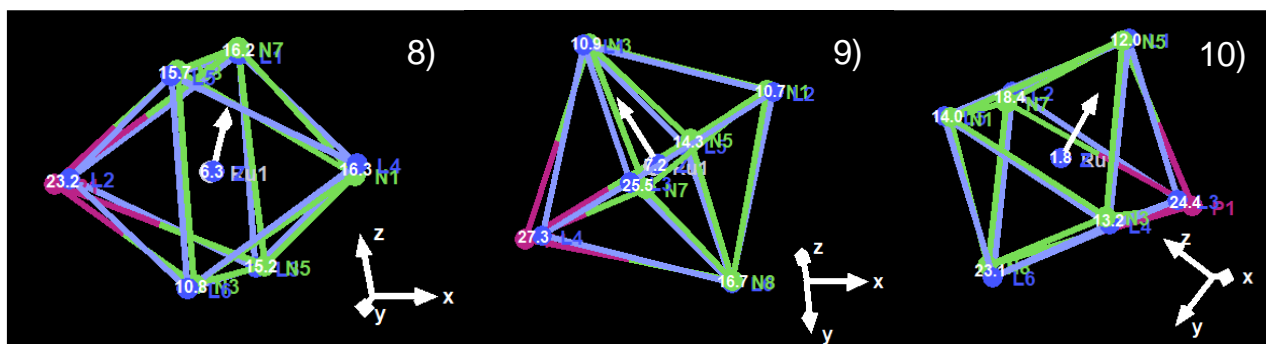


Figure S71. Deviation of the real polyhedron (green and violet) from the ideal octahedron (blue) in complexes **8**, **9** and **10**.

Table S4. Hydrogen bonds for **8**·H₂O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(7)-H(7A)...O(4)#1	0.91	2.13	3.005(13)	160.4
N(7)-H(7A)...O(40)#1	0.91	2.13	3.01(5)	161.1
N(7)-H(7B)...O(1)#1	0.91	2.41	3.168(7)	141.1
N(8)-H(8B)...O(30)	0.91	1.98	2.856(11)	160.0
N(8)-H(8B)...O(7)	0.91	2.34	3.19(3)	155.3
N(8)-H(8B)...O(12)	0.91	2.31	3.020(14)	134.6
O(101)-H(101)...O(2)	0.912(15)	2.040(16)	2.951(8)	177(10)
O(101)-H(102)...O(30)	0.87(2)	2.16(4)	2.808(12)	130(4)
O(101)-H(102)...O(7)	0.87(2)	2.00(2)	2.58(3)	123(3)

Symmetry transformations used to generate equivalent atoms: #1 x,y+1,z.

Table S5. Hydrogen bonds for **9**·solv [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(8)-H(8A)...O(2)#1	0.91	2.40	3.046(13)	127.9

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1,z-1/2.

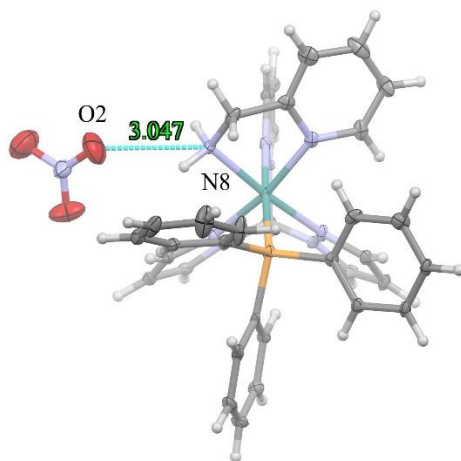


Figure S72. View of hydrogen bonding between N8 of the coordinated 2-picolyamine and O2 of nitrate anion in **9**.

6. DFT Calculations

All the intermediates and the Transition States have been optimized M062X-DFT level of theory [9] with the inclusion of the dispersion forces [10] within the Gaussian 16 software [11] and validated as minima and/or transition states by computed vibrational frequencies. All the calculations were based on the CPCM model [12,13] for the 2-propanol used in the experiments. The effective Stuttgart/Dresden core potential (SDD) [14] was adopted for the ruthenium atom, while for all the other atomic species the basis set was def2tzvp [15]. The calculated reaction pathway (relative free energy, kcal mol⁻¹) is shown in Figure S73. All the Transition States have been firstly localized on the Potential Energy Surface through *ad-hoc* relaxed scans along one reaction coordinate. Once localized, the structures were then optimized as Transition States and the frequency calculations were performed. Cartesian coordinates and free energies of all the structures optimized at M062X-DFT level of theory are listed below (for figures see manuscript).

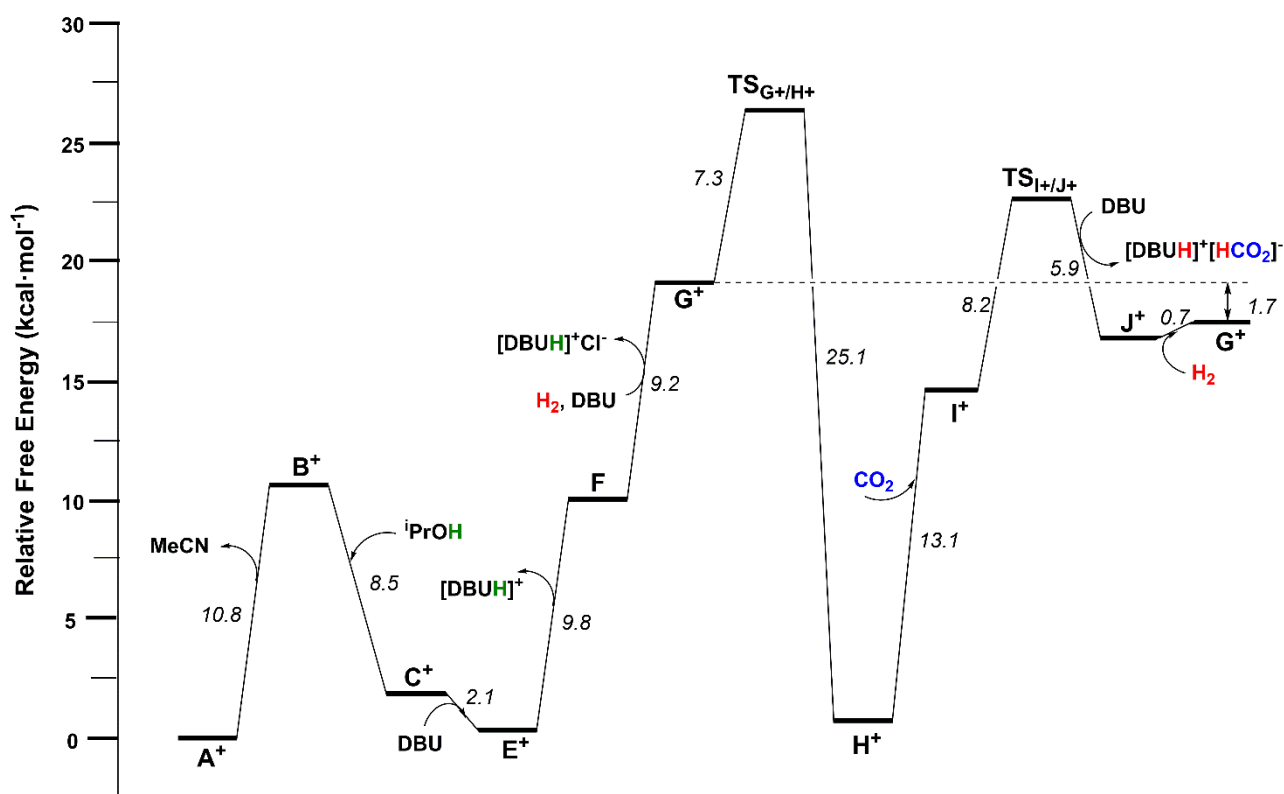
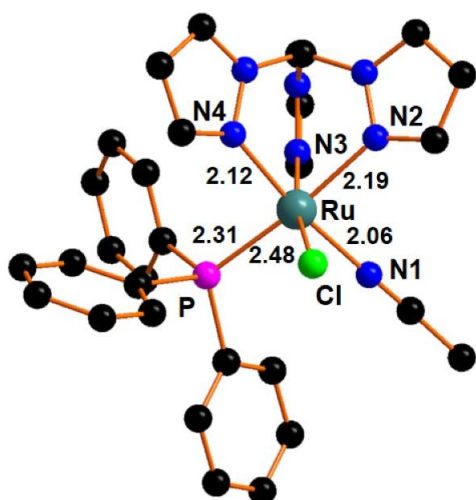


Figure S73. Free energy pathway (kcal mol⁻¹) for the entire process, starting from pre-catalyst A⁺.

Compound A⁺



Cartesian Coordinates

Ru 0.7317 0.5538 -0.4981

Cl 0.3624 0.8590 -2.9283

N 1.4502 -1.4251 -0.7717

N 2.5842 -1.7687 -0.1298

N 1.4060 0.4057 1.4993

N 2.5426 -0.2768 1.7305

N 2.8423 1.0509 -0.8580

N 3.7570 0.2959 -0.2287

C 3.3233 -0.7847 0.6269

H 4.2054 -1.2698 1.0344

C 1.0891 -2.4887 -1.4693

H 0.1987 -2.4537 -2.0761

C 2.0019 -3.5390 -1.2757

H 1.9695 -4.5232 -1.7064

C 2.9485 -3.0390 -0.4197

H 3.8406 -3.4710 0.0014

C	1.0007	0.8455	2.6771
H	0.0869	1.4101	2.7576
C	1.8871	0.4453	3.6891
H	1.8155	0.6479	4.7423
C	2.8648	-0.2675	3.0447
H	3.7530	-0.7598	3.4031
C	3.5195	1.9212	-1.5815
H	2.9877	2.6363	-2.1875
C	4.9031	1.7276	-1.4181
H	5.7037	2.2802	-1.8757
C	5.0164	0.6749	-0.5460
H	5.8724	0.1699	-0.1312
N	0.2855	2.5578	-0.2761
P	-1.4053	-0.1666	-0.0071
C	-1.5263	-0.9138	1.6612
C	-0.5653	-1.8620	2.0247
H	0.2201	-2.1322	1.3280
C	-0.6055	-2.4700	3.2680
H	0.1459	-3.2028	3.5319
C	-1.6042	-2.1312	4.1753
H	-1.6307	-2.5966	5.1519
C	-2.5672	-1.1994	3.8213
H	-3.3524	-0.9369	4.5180
C	-2.5344	-0.5980	2.5667
H	-3.3011	0.1191	2.3056

C	-2.0772	-1.4939	-1.0752
C	-2.4334	-2.7446	-0.5730
H	-2.3684	-2.9523	0.4859
C	-2.8722	-3.7485	-1.4288
H	-3.1370	-4.7161	-1.0231
C	-2.9707	-3.5122	-2.7917
H	-3.3091	-4.2960	-3.4568
C	-2.6379	-2.2613	-3.2984
H	-2.7203	-2.0644	-4.3594
C	-2.1914	-1.2606	-2.4487
H	-1.9122	-0.2988	-2.8558
C	-2.7107	1.1128	0.0006
C	-2.5488	2.2000	0.8634
H	-1.6822	2.2525	1.5107
C	-3.4940	3.2106	0.9183
H	-3.3546	4.0407	1.5987
C	-4.6175	3.1544	0.1002
H	-5.3550	3.9454	0.1362
C	-4.7919	2.0769	-0.7539
H	-5.6683	2.0205	-1.3861
C	-3.8474	1.0566	-0.8007
H	-4.0118	0.2177	-1.4624
C	0.0663	3.6765	-0.2127
C	-0.2499	5.0899	-0.1194
H	-1.1521	5.2906	-0.6948

H -0.4170 5.3522 0.9238

H 0.5759 5.6766 -0.5166

Free Energy: -2439.074272 hartrees

Compound **CH₃CN**

Cartesian Coordinates

N -1.4269 -0.0002 -0.0000

C -0.2806 0.0004 0.0001

C 1.1755 -0.0001 -0.0000

H 1.5391 -1.0227 -0.0748

H 1.5396 0.5757 -0.8482

H 1.5398 0.4463 0.9228

Free Energy: -132.733441 hartrees

Compound **Cl⁻**

Cartesian Coordinates

Cl 0.0000 0.0000 0.0000

Free Energy: -460.382503 hartrees

Compound **PPh₃**

Cartesian Coordinates

P	0.0022	0.0013	-1.2605
C	-1.1122	1.2077	-0.4412
C	-1.1683	2.4892	-0.9920
H	-0.5845	2.7185	-1.8768
C	-1.9603	3.4739	-0.4185
H	-1.9887	4.4643	-0.8543
C	-2.7229	3.1836	0.7062
H	-3.3474	3.9476	1.1511
C	-2.6852	1.9081	1.2539
H	-3.2788	1.6761	2.1289
C	-1.8823	0.9261	0.6864
H	-1.8557	-0.0625	1.1279
C	1.6036	0.3611	-0.4409
C	1.7408	1.1468	0.7024
H	0.8687	1.6026	1.1547
C	2.9924	1.3510	1.2704
H	3.0853	1.9645	2.1574
C	4.1196	0.7673	0.7073
H	5.0932	0.9259	1.1526
C	3.9940	-0.0153	-0.4340
H	4.8691	-0.4677	-0.8822
C	2.7453	-0.2085	-1.0080
H	2.6549	-0.8087	-1.9067
C	-0.4892	-1.5671	-0.4449
C	-1.6045	-2.2252	-0.9686

H	-2.1188	-1.8080	-1.8276
C	-2.0639	-3.4040	-0.4004
H	-2.9336	-3.8986	-0.8134
C	-1.4003	-3.9537	0.6906
H	-1.7523	-4.8776	1.1311
C	-0.2814	-3.3164	1.2083
H	0.2417	-3.7414	2.0555
C	0.1705	-2.1275	0.6467
H	1.0404	-1.6371	1.0657

Free Energy: -460.382503 hartrees

Compound **2-propanol**

Cartesian Coordinates

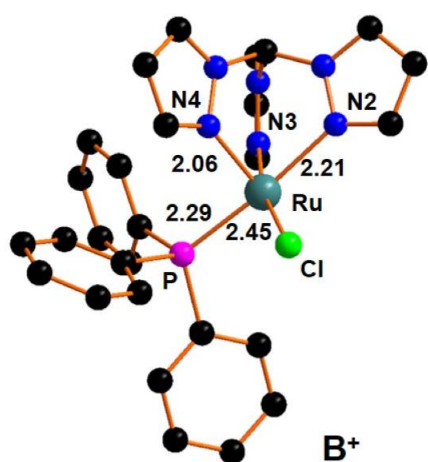
O	-0.0001	1.3576	-0.2309
H	-0.0004	2.0164	0.4675
C	-0.0000	0.0493	0.3535
C	1.2582	-0.6793	-0.0830
C	-1.2581	-0.6794	-0.0830
H	-0.0000	0.1447	1.4425
H	2.1472	-0.1378	0.2408
H	1.2889	-1.6853	0.3376
H	1.2782	-0.7592	-1.1719
H	-2.1471	-0.1381	0.2408

H -1.2781 -0.7594 -1.1719

H -1.2886 -1.6854 0.3376

Free Energy: -194.262179 hartrees

Compound **B⁺**



Cartesian Coordinates

Ru 0.7245 -0.4490 -0.8156

Cl 0.2095 -2.7352 -1.5241

N 1.3976 -0.9032 1.0543

N 2.5352 -0.3244 1.4906

N 1.4230 1.5171 -0.4943

N 2.5664 1.6731 0.1965

N 2.8441 -0.8077 -1.3488

N 3.7578 -0.2469 -0.5394

C 3.3172 0.5126 0.6086

H 4.1932 0.8487 1.1560

C 1.0135 -1.7358 2.0083

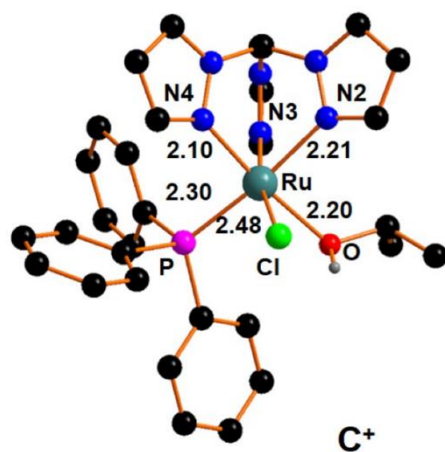
H	0.1183	-2.3222	1.8817
C	1.9163	-1.6942	3.0828
H	1.8651	-2.2520	4.0000
C	2.8787	-0.7915	2.7128
H	3.7702	-0.4435	3.2065
C	1.0387	2.7321	-0.8443
H	0.1234	2.8712	-1.3962
C	1.9504	3.6919	-0.3770
H	1.9005	4.7585	-0.5006
C	2.9180	2.9768	0.2805
H	3.8150	3.2794	0.7939
C	3.5252	-1.4685	-2.2660
H	2.9971	-2.0130	-3.0312
C	4.9078	-1.3334	-2.0478
H	5.7096	-1.7542	-2.6270
C	5.0179	-0.5475	-0.9290
H	5.8724	-0.1831	-0.3840
P	-1.3896	0.0152	-0.0781
C	-1.4838	1.6293	0.7720
C	-0.5855	1.8820	1.8135
H	0.1095	1.1114	2.1305
C	-0.5663	3.1135	2.4451
H	0.1330	3.2937	3.2511
C	-1.4364	4.1188	2.0334
H	-1.4146	5.0860	2.5183

C	-2.3283	3.8781	1.0003
H	-3.0070	4.6558	0.6756
C	-2.3567	2.6359	0.3730
H	-3.0553	2.4654	-0.4360
C	-2.1080	-1.1561	1.1269
C	-2.3495	-0.8205	2.4568
H	-2.1723	0.1847	2.8129
C	-2.8242	-1.7775	3.3472
H	-3.0023	-1.5041	4.3789
C	-3.0708	-3.0717	2.9153
H	-3.4376	-3.8159	3.6101
C	-2.8536	-3.4076	1.5833
H	-3.0552	-4.4126	1.2362
C	-2.3745	-2.4581	0.6943
H	-2.1926	-2.7304	-0.3369
C	-2.6622	0.1186	-1.3762
C	-2.2908	0.5099	-2.6619
H	-1.2531	0.7138	-2.8984
C	-3.2497	0.6540	-3.6560
H	-2.9505	0.9568	-4.6507
C	-4.5859	0.4067	-3.3730
H	-5.3329	0.5153	-4.1484
C	-4.9638	0.0187	-2.0934
H	-6.0047	-0.1731	-1.8684
C	-4.0076	-0.1240	-1.0985

H -4.3111 -0.4240 -0.1032

Free Energy: -2306.323521 hartrees

Compound C^+



Cartesian Coordinates

Ru 0.7297 0.2640 -0.5134

Cl 0.4253 0.6633 -2.9396

N 1.0723 -1.7972 -0.6523

N 2.1097 -2.3073 0.0428

N 1.3203 0.1171 1.5056

N 2.3344 -0.7159 1.8022

N 2.9072 0.3263 -0.8875

N 3.6579 -0.5201 -0.1639

C 3.0165 -1.4333 0.7533

H 3.7843 -2.0493 1.2122

C 0.5413 -2.8117 -1.3140

H -0.3123 -2.6488 -1.9515

C 1.2419 -3.9986 -1.0416

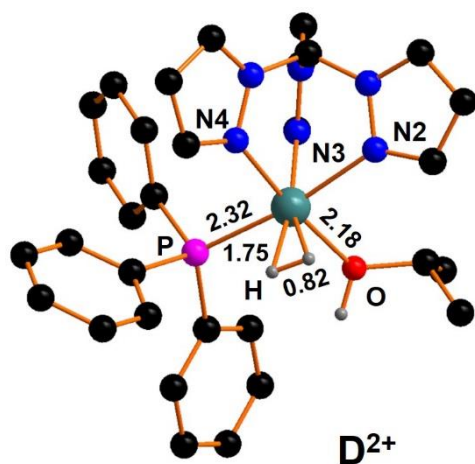
H	1.0397	-4.9811	-1.4278
C	2.2420	-3.6363	-0.1782
H	3.0289	-4.2019	0.2918
C	0.9497	0.6574	2.6541
H	0.1147	1.3378	2.6865
C	1.7397	0.1757	3.7089
H	1.6696	0.4309	4.7506
C	2.6168	-0.7015	3.1248
H	3.4085	-1.3082	3.5308
C	3.7417	0.9496	-1.6984
H	3.3618	1.6761	-2.3977
C	5.0587	0.5023	-1.4944
H	5.9498	0.8264	-2.0009
C	4.9642	-0.4457	-0.5077
H	5.7030	-1.0662	-0.0293
P	-1.5011	-0.0306	-0.0373
C	-1.7789	-0.6589	1.6605
C	-1.0336	-1.7626	2.0865
H	-0.3306	-2.2360	1.4103
C	-1.1816	-2.2641	3.3683
H	-0.5977	-3.1199	3.6810
C	-2.0711	-1.6609	4.2522
H	-2.1798	-2.0440	5.2584
C	-2.8188	-0.5701	3.8378
H	-3.5169	-0.0993	4.5175

C	-2.6795	-0.0738	2.5449
H	-3.2747	0.7762	2.2381
C	-2.3622	-1.2705	-1.0725
C	-2.8955	-2.4465	-0.5492
H	-2.8627	-2.6411	0.5136
C	-3.4731	-3.3923	-1.3891
H	-3.8755	-4.3042	-0.9677
C	-3.5349	-3.1684	-2.7561
H	-3.9818	-3.9069	-3.4088
C	-3.0271	-1.9863	-3.2835
H	-3.0818	-1.7977	-4.3477
C	-2.4430	-1.0452	-2.4497
H	-2.0351	-0.1367	-2.8711
C	-2.5842	1.4365	-0.1221
C	-2.1739	2.5896	0.5502
H	-1.2195	2.6059	1.0585
C	-2.9778	3.7184	0.5725
H	-2.6479	4.6028	1.1021
C	-4.2015	3.7128	-0.0867
H	-4.8276	4.5954	-0.0760
C	-4.6194	2.5709	-0.7542
H	-5.5742	2.5570	-1.2631
C	-3.8189	1.4346	-0.7674
H	-4.1681	0.5484	-1.2795
O	0.6213	2.4635	-0.5240

H	0.4233	2.6105	-1.4625
C	1.6819	3.3520	-0.0920
C	1.2186	4.0774	1.1535
C	2.0267	4.3068	-1.2162
H	2.5432	2.7236	0.1442
H	0.9748	3.3747	1.9494
H	2.0112	4.7328	1.5150
H	0.3377	4.6825	0.9317
H	2.3175	3.7679	-2.1193
H	1.1675	4.9399	-1.4482
H	2.8557	4.9481	-0.9192

Free Energy: -2500.599246 hartrees

Compound D^{2+}



Cartesian Coordinates

Ru	0.7104	0.3026	-0.6892
N	1.1178	-1.7548	-0.7871

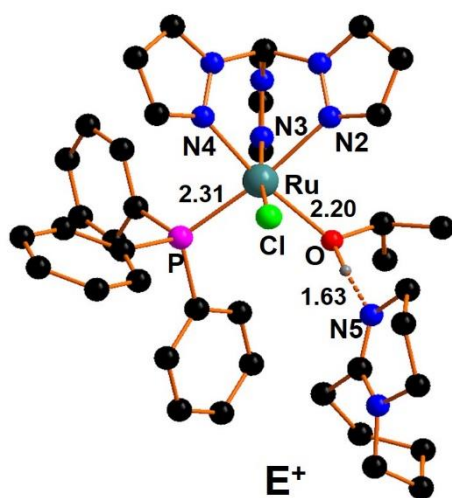
N	2.1585	-2.2237	-0.0686
N	1.3727	0.2674	1.3203
N	2.3627	-0.5811	1.6477
N	2.8975	0.4207	-1.0631
N	3.6624	-0.4100	-0.3307
C	3.0504	-1.3148	0.6140
H	3.8347	-1.9030	1.0812
C	0.5925	-2.8062	-1.3978
H	-0.2640	-2.6888	-2.0413
C	1.3003	-3.9712	-1.0686
H	1.1049	-4.9721	-1.4076
C	2.2982	-3.5596	-0.2242
H	3.0890	-4.0961	0.2727
C	1.0304	0.8810	2.4404
H	0.2333	1.6048	2.4416
C	1.8131	0.4264	3.5104
H	1.7619	0.7367	4.5381
C	2.6594	-0.5049	2.9637
H	3.4407	-1.1093	3.3932
C	3.7312	1.0587	-1.8684
H	3.3560	1.7868	-2.5680
C	5.0523	0.6398	-1.6524
H	5.9399	0.9817	-2.1529
C	4.9681	-0.3054	-0.6627
H	5.7165	-0.9051	-0.1725

P	-1.5060	-0.0604	-0.0887
C	-1.6717	-0.7011	1.6091
C	-0.8462	-1.7567	2.0075
H	-0.1388	-2.1905	1.3113
C	-0.9282	-2.2673	3.2913
H	-0.2833	-3.0847	3.5855
C	-1.8332	-1.7251	4.1982
H	-1.8909	-2.1165	5.2052
C	-2.6642	-0.6873	3.8070
H	-3.3771	-0.2678	4.5043
C	-2.5901	-0.1782	2.5146
H	-3.2517	0.6269	2.2252
C	-2.3202	-1.3099	-1.1366
C	-2.8318	-2.4908	-0.6056
H	-2.8134	-2.6668	0.4611
C	-3.3624	-3.4634	-1.4457
H	-3.7474	-4.3810	-1.0213
C	-3.3968	-3.2604	-2.8165
H	-3.8053	-4.0209	-3.4685
C	-2.9113	-2.0723	-3.3523
H	-2.9480	-1.8994	-4.4195
C	-2.3732	-1.1056	-2.5187
H	-2.0102	-0.1834	-2.9576
C	-2.5999	1.3969	-0.1487
C	-2.2786	2.5079	0.6376

H	-1.4033	2.4916	1.2739
C	-3.0794	3.6387	0.6242
H	-2.8168	4.4882	1.2405
C	-4.2154	3.6746	-0.1756
H	-4.8403	4.5576	-0.1896
C	-4.5498	2.5725	-0.9476
H	-5.4393	2.5891	-1.5632
C	-3.7504	1.4360	-0.9338
H	-4.0387	0.5830	-1.5315
O	0.4698	2.4595	-0.4820
H	-0.3445	2.8358	-0.8449
C	1.5227	3.4574	-0.5167
C	1.2592	4.4823	0.5667
C	1.6030	4.0688	-1.8994
H	2.4282	2.8972	-0.2864
H	1.2176	4.0080	1.5466
H	2.0565	5.2255	0.5739
H	0.3138	4.9967	0.3809
H	1.6851	3.3012	-2.6687
H	0.7077	4.6615	-2.1016
H	2.4687	4.7270	-1.9678
H	0.6632	0.4695	-2.4336
H	-0.0992	0.2396	-2.2381

Free energy: -2041.341882 hartrees

Compound E⁺



Cartesian Coordinates

Ru 0.8705 -0.7713 0.1603

Cl -0.4394 -1.0829 2.2343

N 2.6189 -0.8222 1.3037

N 3.6471 -1.5705 0.8590

N 2.1136 -0.8518 -1.5606

N 3.2134 -1.6245 -1.4847

N 1.1884 -2.9618 0.1882

N 2.4370 -3.3825 -0.0795

C 3.4812 -2.4113 -0.3062

H 4.4131 -2.9446 -0.4681

C 3.0092 -0.3057 2.4554

H 2.3392 0.3356 3.0049

C 4.3169 -0.7218 2.7618

H 4.9020 -0.4611 3.6250

C 4.6885 -1.5368 1.7244

H	5.5909	-2.0916	1.5301
C	2.1490	-0.2997	-2.7617
H	1.3860	0.3970	-3.0622
C	3.2801	-0.7227	-3.4758
H	3.5716	-0.4402	-4.4710
C	3.9395	-1.5708	-2.6246
H	4.8499	-2.1362	-2.7315
C	0.5075	-4.0410	0.5218
H	-0.5259	-3.9499	0.8108
C	1.3244	-5.1844	0.4633
H	1.0484	-6.2022	0.6720
C	2.5578	-4.7206	0.0857
H	3.4971	-5.2213	-0.0782
P	0.8281	1.5270	0.1603
C	2.2269	2.2817	-0.7670
C	3.5108	1.7510	-0.6167
H	3.6759	0.9012	0.0318
C	4.5920	2.3032	-1.2852
H	5.5778	1.8764	-1.1531
C	4.4074	3.3944	-2.1262
H	5.2485	3.8208	-2.6569
C	3.1396	3.9347	-2.2780
H	2.9856	4.7880	-2.9256
C	2.0568	3.3865	-1.5989
H	1.0781	3.8283	-1.7300

C	0.9664	2.3297	1.7974
C	2.0765	3.0837	2.1729
H	2.8875	3.2509	1.4769
C	2.1591	3.6258	3.4506
H	3.0304	4.2035	3.7302
C	1.1297	3.4306	4.3593
H	1.1945	3.8536	5.3534
C	0.0107	2.6942	3.9866
H	-0.8004	2.5448	4.6875
C	-0.0688	2.1430	2.7171
H	-0.9347	1.5566	2.4399
C	-0.6022	2.3667	-0.6082
C	-0.9332	1.9718	-1.9043
H	-0.4141	1.1367	-2.3479
C	-1.9272	2.6198	-2.6174
H	-2.1648	2.2994	-3.6241
C	-2.6277	3.6661	-2.0272
H	-3.4147	4.1696	-2.5737
C	-2.3160	4.0598	-0.7343
H	-2.8569	4.8741	-0.2698
C	-1.3000	3.4220	-0.0288
H	-1.0548	3.7624	0.9679
O	-0.9642	-1.0331	-1.0237
H	-1.8565	-1.0604	-0.4986
C	-1.0276	-1.8922	-2.1699

C	-1.4751	-1.1080	-3.3953
C	-1.9584	-3.0728	-1.9389
H	-0.0136	-2.2690	-2.3254
H	-0.7336	-0.3762	-3.7129
H	-1.6509	-1.7857	-4.2318
H	-2.4078	-0.5833	-3.1707
H	-1.7230	-3.5859	-1.0086
H	-2.9970	-2.7408	-1.8965
H	-1.8551	-3.7829	-2.7598
C	-4.1691	-0.3118	0.3538
C	-3.4182	-2.4654	1.0041
C	-4.3136	-2.3124	2.2208
H	-3.8327	-3.2239	0.3316
C	-5.6098	-1.6526	1.7914
H	-3.8151	-1.6841	2.9627
H	-6.2349	-1.4135	2.6524
C	-3.9882	0.9602	-0.4300
C	-6.4066	0.5193	0.8715
N	-3.2529	-1.2156	0.2719
N	-5.3061	-0.4093	1.0964
H	-2.4245	-2.7982	1.3055
H	-4.5170	-3.2809	2.6768
H	-6.1815	-2.3252	1.1407
C	-7.1205	0.2823	-0.4612
C	-4.9867	1.1142	-1.6079

C	-6.1337	0.1013	-1.6155
H	-4.0635	1.8081	0.2520
H	-2.9689	0.9491	-0.8047
H	-4.4305	1.0131	-2.5415
H	-5.3956	2.1278	-1.6042
H	-5.7130	-0.9088	-1.5806
H	-6.6711	0.1725	-2.5624
H	-6.0277	1.5403	0.9111
H	-7.1012	0.4119	1.7041
H	-7.7649	-0.5967	-0.3892
H	-7.7699	1.1403	-0.6530

Free energy: -2962.445615 hartrees

Compound **DBU**

Cartesian Coordinates

C	0.2784	-0.7647	-0.3714
C	2.4384	-0.8215	0.5852
C	2.6672	0.5503	-0.0309
H	2.3918	-0.7309	1.6761
C	1.3844	1.3519	0.0803
H	2.9298	0.4452	-1.0861
H	1.4708	2.3107	-0.4328
C	-0.9908	-1.4557	-0.8105

C	-0.9314	1.3286	-0.8004
N	1.2219	-1.4798	0.1221
N	0.3027	0.6017	-0.5390
H	3.2830	-1.4790	0.3697
H	3.4851	1.0695	0.4692
H	1.1594	1.5586	1.1352
C	-1.8682	1.3834	0.4090
C	-2.2144	-1.1349	0.0923
C	-2.0065	0.0167	1.0794
H	-1.2017	-1.1885	-1.8468
H	-0.7819	-2.5220	-0.7917
H	-2.4634	-2.0299	0.6631
H	-3.0817	-0.9169	-0.5357
H	-1.1127	-0.1872	1.6769
H	-2.8415	0.0422	1.7816
H	-1.4467	0.8669	-1.6421
H	-0.6584	2.3350	-1.1189
H	-1.5026	2.1129	1.1354
H	-2.8448	1.7361	0.0668

Free Energy: -461.843035 hartrees

Compound [DBUH]⁺

Cartesian Coordinates

H	1.2039	-2.3689	0.1330
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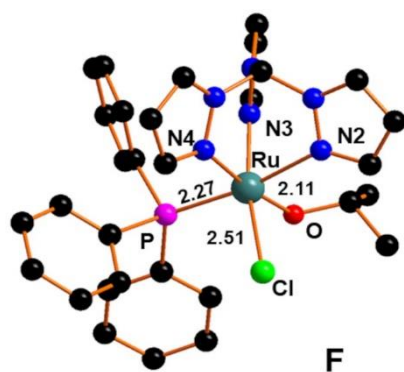
C	0.2460	-0.6899	-0.3505
C	2.5160	-0.7499	0.5939
C	2.6791	0.6004	-0.0759
H	2.4671	-0.6468	1.6790
C	1.4005	1.4025	0.0745
H	2.9008	0.4626	-1.1349
H	1.4471	2.3175	-0.5121
C	-0.9669	-1.4488	-0.8010
C	-0.9716	1.3493	-0.7688
N	1.2799	-1.3640	0.1151
N	0.2555	0.6264	-0.4156
H	3.3380	-1.4177	0.3483
H	3.5062	1.1422	0.3776
H	1.2255	1.6743	1.1186
C	-1.9707	1.3624	0.3872
C	-2.2363	-1.1636	0.0500
C	-2.1107	-0.0098	1.0458
H	-1.1356	-1.1929	-1.8473
H	-0.7288	-2.5098	-0.7777
H	-2.4801	-2.0699	0.6019
H	-3.0707	-0.9716	-0.6262
H	-1.2551	-0.1921	1.7029
H	-2.9880	-0.0066	1.6927
H	-1.4095	0.8826	-1.6496
H	-0.6815	2.3580	-1.0526

H -1.6677 2.0982 1.1339

H -2.9320 1.6880 -0.0149

Free Energy: -462.300108 hartrees

Compound F



Cartesian Coordinates

Ru 0.6811 0.3562 -0.5549

Cl 0.2608 0.4807 -3.0316

N 1.0805 -1.7654 -0.6864

N 2.0900 -2.2384 0.0718

N 1.3890 0.3238 1.4064

N 2.3568 -0.5443 1.7463

N 2.8999 0.3694 -0.9996

N 3.6381 -0.4732 -0.2544

C 3.0028 -1.3284 0.7240

H 3.7757 -1.9236 1.2013

C 0.5674 -2.8186 -1.2978

H -0.2680 -2.6941 -1.9672

C 1.2544 -3.9919 -0.9340

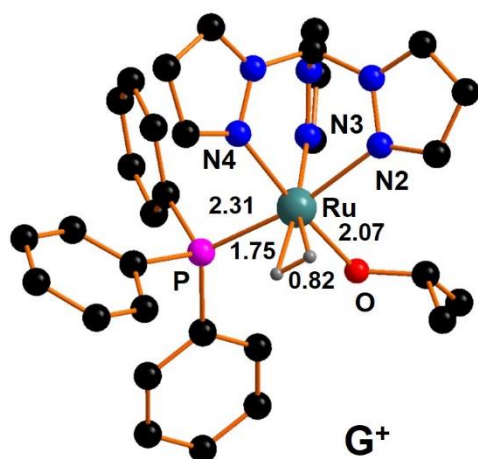
H	1.0601	-4.9960	-1.2655
C	2.2296	-3.5790	-0.0654
H	3.0028	-4.1142	0.4597
C	1.1498	1.0527	2.4783
H	0.3926	1.8169	2.4309
C	1.9847	0.6540	3.5388
H	2.0141	1.0524	4.5370
C	2.7522	-0.3612	3.0304
H	3.5352	-0.9610	3.4629
C	3.7393	0.9050	-1.8658
H	3.3795	1.6205	-2.5848
C	5.0413	0.4046	-1.6813
H	5.9293	0.6599	-2.2310
C	4.9347	-0.4828	-0.6423
H	5.6585	-1.1116	-0.1516
P	-1.4817	0.0018	0.0436
C	-1.6070	-0.3979	1.8269
C	-0.8586	-1.4763	2.3117
H	-0.2936	-2.0944	1.6207
C	-0.8142	-1.7573	3.6661
H	-0.2330	-2.5981	4.0226
C	-1.5031	-0.9495	4.5666
H	-1.4612	-1.1608	5.6272
C	-2.2357	0.1298	4.0992
H	-2.7677	0.7673	4.7936

C	-2.2907	0.4033	2.7348
H	-2.8602	1.2556	2.3875
C	-2.2837	-1.4386	-0.7733
C	-2.6267	-2.6242	-0.1307
H	-2.4797	-2.7371	0.9341
C	-3.1687	-3.6858	-0.8493
H	-3.4244	-4.6029	-0.3344
C	-3.3829	-3.5698	-2.2141
H	-3.8004	-4.3976	-2.7725
C	-3.0691	-2.3778	-2.8594
H	-3.2450	-2.2726	-3.9223
C	-2.5258	-1.3217	-2.1448
H	-2.2628	-0.4052	-2.6573
C	-2.8007	1.2461	-0.2112
C	-2.4953	2.5306	-0.6507
H	-1.4541	2.7934	-0.8051
C	-3.5172	3.4559	-0.8520
H	-3.2750	4.4536	-1.1962
C	-4.8373	3.1068	-0.6138
H	-5.6285	3.8287	-0.7713
C	-5.1462	1.8228	-0.1725
H	-6.1754	1.5442	0.0138
C	-4.1344	0.8975	0.0227
H	-4.3815	-0.1038	0.3575
O	0.4506	2.4226	-0.1978

C	1.5782	3.2272	-0.2253
C	1.4100	4.3913	0.7518
C	1.8364	3.7673	-1.6352
H	2.4770	2.6676	0.0926
H	1.2847	4.0205	1.7707
H	2.2713	5.0640	0.7307
H	0.5179	4.9648	0.4842
H	1.7766	2.9514	-2.3562
H	1.0586	4.4921	-1.8945
H	2.8094	4.2593	-1.7218

Free Energy: -2500.129818 hartrees

Compound **G⁺**



Cartesian Coordinates

Ru	0.7265	0.4464	-0.6754
N	1.2257	-1.6618	-0.8335
N	2.2171	-2.1162	-0.0427

N	1.3329	0.3699	1.3446
N	2.2988	-0.4879	1.7087
N	2.9491	0.5936	-0.9468
N	3.6832	-0.2598	-0.2071
C	3.0463	-1.1913	0.6958
H	3.8237	-1.7655	1.1916
C	0.7652	-2.7225	-1.4768
H	-0.0457	-2.6176	-2.1795
C	1.4635	-3.8799	-1.0941
H	1.3098	-4.8847	-1.4436
C	2.3907	-3.4510	-0.1803
H	3.1523	-3.9735	0.3737
C	0.9423	0.9821	2.4458
H	0.1572	1.7185	2.3926
C	1.6722	0.5125	3.5506
H	1.5771	0.8157	4.5775
C	2.5383	-0.4202	3.0388
H	3.2972	-1.0303	3.4985
C	3.8181	1.2562	-1.6902
H	3.4739	2.0149	-2.3728
C	5.1306	0.8296	-1.4309
H	6.0395	1.1881	-1.8790
C	5.0032	-0.1451	-0.4757
H	5.7289	-0.7582	0.0314
P	-1.4661	-0.0408	-0.1253

C	-1.5808	-0.7435	1.5614
C	-0.7610	-1.8256	1.8982
H	-0.1254	-2.2812	1.1482
C	-0.7552	-2.3333	3.1859
H	-0.1156	-3.1720	3.4289
C	-1.5657	-1.7629	4.1629
H	-1.5556	-2.1536	5.1720
C	-2.3868	-0.6958	3.8369
H	-3.0237	-0.2494	4.5893
C	-2.3978	-0.1881	2.5408
H	-3.0413	0.6497	2.3068
C	-2.1747	-1.3398	-1.2014
C	-2.5785	-2.5854	-0.7309
H	-2.5352	-2.8138	0.3250
C	-3.0372	-3.5558	-1.6159
H	-3.3382	-4.5236	-1.2368
C	-3.1094	-3.2862	-2.9738
H	-3.4614	-4.0440	-3.6612
C	-2.7375	-2.0328	-3.4487
H	-2.8069	-1.8070	-4.5045
C	-2.2726	-1.0689	-2.5686
H	-1.9962	-0.0948	-2.9558
C	-2.7632	1.2394	-0.1273
C	-2.4591	2.5124	0.3588
H	-1.4330	2.7502	0.6104

C	-3.4593	3.4696	0.4693
H	-3.2166	4.4556	0.8445
C	-4.7626	3.1687	0.0956
H	-5.5389	3.9184	0.1800
C	-5.0688	1.9033	-0.3880
H	-6.0827	1.6620	-0.6791
C	-4.0753	0.9396	-0.4956
H	-4.3306	-0.0458	-0.8633
O	0.3732	2.4688	-0.3821
C	1.3336	3.4176	-0.7081
C	1.0414	4.6972	0.0735
C	1.3502	3.7195	-2.2080
H	2.3429	3.0839	-0.4136
H	1.0650	4.4970	1.1461
H	1.7681	5.4810	-0.1513
H	0.0444	5.0636	-0.1850
H	1.4780	2.8065	-2.7934
H	0.3951	4.1646	-2.4994
H	2.1515	4.4132	-2.4747
H	0.7109	0.6531	-2.4102
H	-0.0776	0.5153	-2.2199

Free Energy: -2040.891614 hartrees

Compound **H₂**

Cartesian Coordinates

H 0.0000 0.0000 0.0000

H 0.0000 0.0000 0.7405

Free Energy: -1.169909 hartrees

Compound **[DBUH]⁺Cl⁻**

Cartesian Coordinates

H 1.9219 0.2501 0.0310

C -0.0374 0.1005 -0.3989

C 0.9789 2.1110 0.5506

C -0.2080 2.8363 -0.0543

H 0.9075 2.0885 1.6400

C -1.4600 1.9959 0.1205

H -0.0321 3.0078 -1.1172

H -2.2981 2.4328 -0.4193

C 0.1378 -1.3114 -0.8747

C -2.4145 -0.1713 -0.7268

N 1.0155 0.7450 0.0436

N -1.2421 0.6510 -0.4183

H 1.9192 2.5894 0.2831

H -0.3439 3.8019 0.4283

H -1.7369 1.9207 1.1759

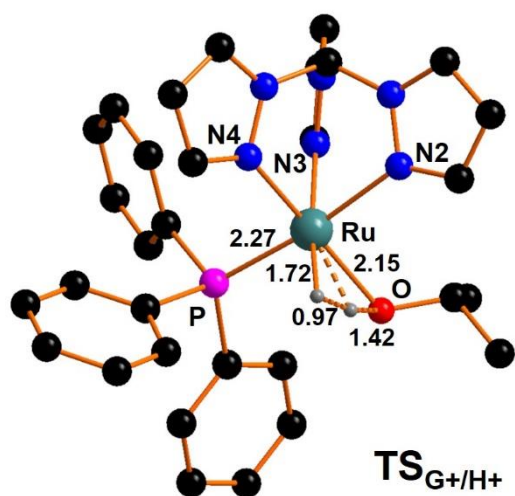
C -2.7826 -1.0979 0.4327

C -0.5793 -2.3538 0.0269

C	-1.5576	-1.7729	1.0495
H	-0.2344	-1.3616	-1.8979
H	1.2064	-1.5145	-0.9117
H	0.1852	-2.9125	0.5657
H	-1.1011	-3.0678	-0.6124
H	-1.0270	-1.0571	1.6848
H	-1.8888	-2.5721	1.7133
H	-2.2096	-0.7489	-1.6265
H	-3.2316	0.5067	-0.9631
H	-3.3144	-0.5365	1.2031
H	-3.4744	-1.8497	0.0474
Cl	3.7573	-0.7511	0.0380

Free Energy: -922.693515 hartrees

Transition State TS_{G^+/H^+}



Imaginary Frequency at -1278 cm^{-1}

Cartesian Coordinates

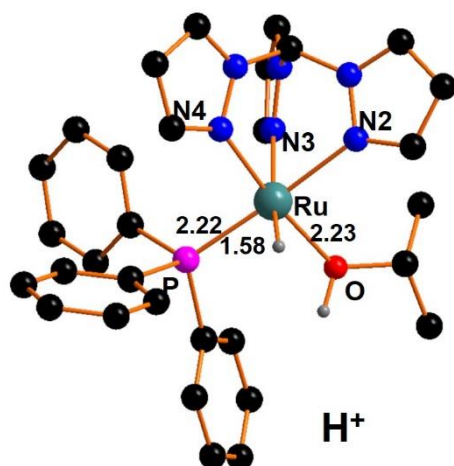
Ru	0.7148	0.4144	-0.5895
N	1.2565	-1.6435	-0.8328
N	2.3339	-2.1012	-0.1660
N	1.3853	0.1625	1.4521
N	2.4696	-0.5976	1.6786
N	2.9042	0.6541	-0.9678
N	3.7228	-0.1835	-0.3070
C	3.1797	-1.1919	0.5735
H	4.0091	-1.7640	0.9781
C	0.7876	-2.6774	-1.5128
H	-0.0871	-2.5617	-2.1316
C	1.5691	-3.8209	-1.2806
H	1.4294	-4.8049	-1.6901
C	2.5542	-3.4120	-0.4200
H	3.3847	-3.9335	0.0250
C	0.9933	0.5961	2.6370
H	0.1176	1.2194	2.7195
C	1.8381	0.1111	3.6485
H	1.7687	0.2917	4.7059
C	2.7737	-0.6504	2.9959
H	3.6192	-1.2150	3.3513
C	3.6871	1.3769	-1.7490
H	3.2576	2.1332	-2.3858
C	5.0328	1.0050	-1.5927
H	5.8920	1.4171	-2.0900

C	5.0152	-0.0028	-0.6632
H	5.8014	-0.5981	-0.2299
P	-1.4522	-0.0751	-0.1268
C	-1.6668	-0.9039	1.4935
C	-0.8587	-2.0052	1.7919
H	-0.1519	-2.3749	1.0590
C	-0.9499	-2.6377	3.0204
H	-0.3179	-3.4901	3.2335
C	-1.8443	-2.1715	3.9787
H	-1.9090	-2.6580	4.9432
C	-2.6538	-1.0841	3.6910
H	-3.3563	-0.7184	4.4285
C	-2.5710	-0.4555	2.4520
H	-3.2131	0.3905	2.2454
C	-2.2115	-1.2428	-1.3103
C	-2.8009	-2.4420	-0.9201
H	-2.8566	-2.7095	0.1266
C	-3.3171	-3.3132	-1.8738
H	-3.7641	-4.2468	-1.5581
C	-3.2607	-2.9877	-3.2206
H	-3.6599	-3.6682	-3.9612
C	-2.6927	-1.7813	-3.6166
H	-2.6527	-1.5167	-4.6651
C	-2.1678	-0.9176	-2.6684
H	-1.7172	0.0144	-2.9869

C	-2.6579	1.2888	-0.0465
C	-2.3084	2.4302	0.6763
H	-1.3125	2.5152	1.0896
C	-3.2192	3.4620	0.8407
H	-2.9383	4.3423	1.4046
C	-4.4856	3.3696	0.2739
H	-5.1946	4.1782	0.3964
C	-4.8385	2.2397	-0.4498
H	-5.8232	2.1619	-0.8917
C	-3.9304	1.1988	-0.6057
H	-4.2228	0.3177	-1.1621
O	0.2593	2.5074	-0.7404
C	1.2344	3.4976	-0.5160
C	0.8846	4.2521	0.7607
C	1.2993	4.4371	-1.7125
H	2.2234	3.0467	-0.3725
H	0.8565	3.5663	1.6098
H	1.6201	5.0305	0.9723
H	-0.0981	4.7188	0.6586
H	1.5344	3.8838	-2.6243
H	0.3302	4.9219	-1.8517
H	2.0575	5.2095	-1.5707
H	0.3212	1.5828	-1.8205
H	0.3188	0.7126	-2.2420

Free Energy: -2040.880020 hartrees

Compound H⁺



Cartesian Coordinates

Ru 0.6683 0.2772 -0.6249

N 1.0965 -1.7887 -0.7858

N 2.2364 -2.2467 -0.2249

N 1.6233 0.1180 1.4438

N 2.6852 -0.6953 1.5408

N 2.8180 0.4149 -1.2483

N 3.6789 -0.3993 -0.6123

C 3.2048 -1.3505 0.3671

H 4.0546 -1.9505 0.6793

C 0.5005 -2.8522 -1.3001

H -0.4426 -2.7416 -1.8090

C 1.2594 -4.0124 -1.0718

H 1.0271 -5.0181 -1.3720

C 2.3656 -3.5852 -0.3872

H	3.2260	-4.1098	-0.0072
C	1.4160	0.5784	2.6630
H	0.5993	1.2573	2.8485
C	2.3605	0.0565	3.5663
H	2.4416	0.2481	4.6211
C	3.1605	-0.7587	2.8076
H	4.0141	-1.3674	3.0543
C	3.5410	1.0655	-2.1427
H	3.0696	1.7781	-2.7987
C	4.8896	0.6737	-2.0831
H	5.7068	1.0305	-2.6835
C	4.9374	-0.2741	-1.0941
H	5.7471	-0.8648	-0.6997
P	-1.4699	-0.0300	-0.0978
C	-1.8177	-0.7361	1.5612
C	-0.9512	-1.7116	2.0560
H	-0.0767	-1.9955	1.4834
C	-1.1956	-2.3238	3.2775
H	-0.5135	-3.0793	3.6457
C	-2.3079	-1.9616	4.0264
H	-2.4958	-2.4323	4.9826
C	-3.1786	-0.9941	3.5427
H	-4.0500	-0.7105	4.1185
C	-2.9383	-0.3895	2.3155
H	-3.6339	0.3531	1.9459

C	-2.4390	-1.1524	-1.1853
C	-3.2591	-2.1591	-0.6782
H	-3.3593	-2.2975	0.3900
C	-3.9488	-3.0092	-1.5360
H	-4.5722	-3.7922	-1.1242
C	-3.8376	-2.8570	-2.9099
H	-4.3733	-3.5203	-3.5764
C	-3.0307	-1.8497	-3.4264
H	-2.9376	-1.7226	-4.4972
C	-2.3315	-1.0109	-2.5716
H	-1.6840	-0.2463	-2.9806
C	-2.4805	1.5032	-0.0844
C	-2.2164	2.4496	0.9107
H	-1.4728	2.2364	1.6695
C	-2.8933	3.6585	0.9383
H	-2.6781	4.3774	1.7182
C	-3.8442	3.9448	-0.0353
H	-4.3723	4.8892	-0.0170
C	-4.1144	3.0139	-1.0269
H	-4.8564	3.2274	-1.7853
C	-3.4383	1.7984	-1.0515
H	-3.6704	1.0810	-1.8273
O	0.4533	2.4696	-0.3474
C	1.4714	3.4651	-0.5790
C	2.5155	3.3182	0.5057

C	0.8224	4.8347	-0.5734
H	1.9157	3.2728	-1.5586
H	2.9402	2.3154	0.5124
H	3.3192	4.0355	0.3387
H	2.0669	3.5135	1.4815
H	0.0592	4.9105	-1.3508
H	0.3579	5.0245	0.3961
H	1.5711	5.6041	-0.7595
H	0.1537	0.3887	-2.1100
H	-0.3629	2.7475	-0.7821

Free Energy: -2040.919991 hartrees

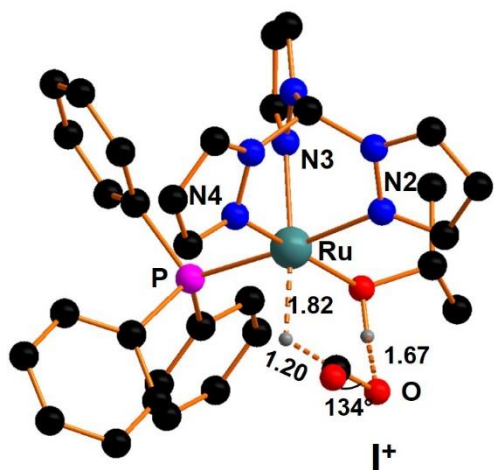
Compound **CO₂**

Cartesian Coordinates

C	0.0000	0.0000	0.0000
O	0.0000	0.0000	1.1540
O	0.0000	0.0000	-1.1540

Free Energy: -188.608159 hartrees

Compound I⁺



Cartesian Coordinates

Ru	0.7036	0.3127	-0.3546
N	1.1604	-1.7019	-0.6998
N	2.2043	-2.2309	-0.0313
N	1.1842	-0.0499	1.6554
N	2.2314	-0.8567	1.9107
N	2.8830	0.5341	-0.6095
N	3.6438	-0.3476	0.0629
C	3.0158	-1.3992	0.8289
H	3.7961	-2.0212	1.2576
C	0.7299	-2.6490	-1.5176
H	-0.1084	-2.4601	-2.1689
C	1.5044	-3.8110	-1.3741
H	1.3890	-4.7425	-1.8976
C	2.4421	-3.5037	-0.4228
H	3.2495	-4.0736	0.0050
C	0.6982	0.2997	2.8340

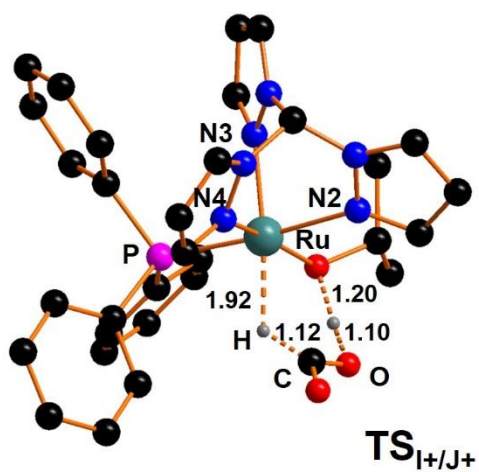
H	-0.1672	0.9385	2.8957
C	1.4436	-0.2814	3.8690
H	1.2856	-0.1801	4.9273
C	2.4172	-1.0152	3.2401
H	3.2170	-1.6280	3.6202
C	3.7227	1.2852	-1.3006
H	3.3420	2.0635	-1.9430
C	5.0496	0.8881	-1.0678
H	5.9450	1.3121	-1.4847
C	4.9587	-0.1659	-0.1950
H	5.7069	-0.7942	0.2578
P	-1.5364	-0.1098	-0.0182
C	-1.8784	-1.0435	1.5147
C	-1.1048	-2.1721	1.8010
H	-0.3349	-2.4944	1.1103
C	-1.3128	-2.8922	2.9651
H	-0.7068	-3.7645	3.1718
C	-2.2908	-2.4874	3.8677
H	-2.4468	-3.0429	4.7831
C	-3.0653	-1.3719	3.5901
H	-3.8307	-1.0538	4.2856
C	-2.8653	-0.6537	2.4155
H	-3.4796	0.2140	2.2141
C	-2.2553	-1.1442	-1.3405
C	-2.7481	-2.4248	-1.1056

H	-2.7807	-2.8249	-0.1015
C	-3.1953	-3.2085	-2.1642
H	-3.5678	-4.2054	-1.9692
C	-3.1639	-2.7170	-3.4600
H	-3.5074	-3.3302	-4.2825
C	-2.6981	-1.4282	-3.6995
H	-2.6853	-1.0309	-4.7058
C	-2.2457	-0.6486	-2.6476
H	-1.8988	0.3587	-2.8478
C	-2.6566	1.3219	0.0902
C	-2.2935	2.3869	0.9165
H	-1.3337	2.3820	1.4152
C	-3.1506	3.4614	1.0953
H	-2.8592	4.2793	1.7412
C	-4.3767	3.4887	0.4417
H	-5.0433	4.3306	0.5757
C	-4.7454	2.4340	-0.3808
H	-5.7011	2.4474	-0.8880
C	-3.8929	1.3505	-0.5524
H	-4.2010	0.5284	-1.1844
O	0.4466	2.4894	-0.2511
C	1.3946	3.4946	0.1720
C	1.8872	3.1759	1.5635
C	0.7056	4.8439	0.0941
H	2.2376	3.4770	-0.5243

H	2.4406	2.2378	1.5863
H	2.5502	3.9724	1.9010
H	1.0483	3.1134	2.2597
H	0.3263	5.0261	-0.9124
H	-0.1311	4.8770	0.7941
H	1.4069	5.6395	0.3460
H	0.1676	0.4738	-2.0900
H	0.3291	2.6263	-1.2289
C	0.8248	1.0695	-2.8968
O	0.7010	2.3022	-2.8279
O	1.3715	0.3221	-3.6844

Free Energy: -2229.506175 hartrees

Transition State $TS_{I+/J+}$



Cartesian Coordinates

Ru	0.7216	0.3430	-0.3322
N	1.2044	-1.6697	-0.7897

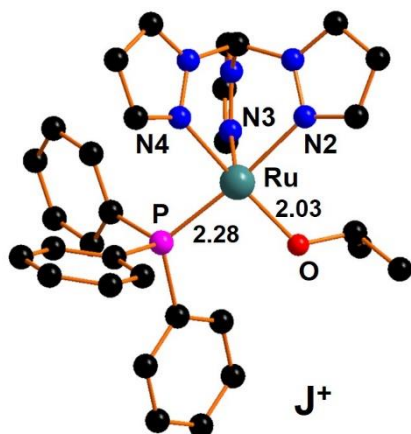
N 2.2415 -2.2229 -0.1333
N 1.1497 -0.1321 1.6319
N 2.1934 -0.9484 1.8740
N 2.9065 0.5871 -0.5377
N 3.6550 -0.3303 0.1004
C 3.0166 -1.4274 0.7908
H 3.7915 -2.0605 1.2127
C 0.7971 -2.5790 -1.6613
H -0.0361 -2.3684 -2.3126
C 1.5808 -3.7400 -1.5643
H 1.4834 -4.6450 -2.1357
C 2.4991 -3.4729 -0.5821
H 3.3043 -4.0566 -0.1689
C 0.6297 0.1582 2.8120
H -0.2368 0.7947 2.8800
C 1.3487 -0.4732 3.8360
H 1.1617 -0.4247 4.8933
C 2.3429 -1.1710 3.1987
H 3.1350 -1.7991 3.5698
C 3.7617 1.3991 -1.1354
H 3.3971 2.2228 -1.7281
C 5.0845 1.0046 -0.8769
H 5.9887 1.4706 -1.2242
C 4.9760 -0.1097 -0.0851
H 5.7165 -0.7562 0.3550

P	-1.5202	-0.1178	-0.0331
C	-1.8529	-1.1853	1.4150
C	-1.0775	-2.3323	1.6089
H	-0.3136	-2.6023	0.8902
C	-1.2751	-3.1384	2.7175
H	-0.6675	-4.0238	2.8514
C	-2.2439	-2.8037	3.6578
H	-2.3915	-3.4270	4.5299
C	-3.0190	-1.6697	3.4729
H	-3.7763	-1.4036	4.1985
C	-2.8290	-0.8646	2.3546
H	-3.4417	0.0184	2.2294
C	-2.2265	-1.0385	-1.4441
C	-2.6582	-2.3582	-1.3486
H	-2.6494	-2.8711	-0.3964
C	-3.0992	-3.0340	-2.4816
H	-3.4259	-4.0619	-2.3958
C	-3.1208	-2.3962	-3.7125
H	-3.4599	-2.9257	-4.5930
C	-2.7155	-1.0692	-3.8113
H	-2.7461	-0.5587	-4.7646
C	-2.2716	-0.3963	-2.6847
H	-1.9818	0.6453	-2.7702
C	-2.6738	1.2699	0.2005
C	-2.2854	2.3270	1.0237

H	-1.2755	2.3626	1.4088
C	-3.1781	3.3460	1.3218
H	-2.8680	4.1614	1.9624
C	-4.4623	3.3234	0.7925
H	-5.1565	4.1216	1.0208
C	-4.8541	2.2760	-0.0302
H	-5.8541	2.2526	-0.4428
C	-3.9663	1.2489	-0.3219
H	-4.2890	0.4296	-0.9512
O	0.4218	2.4508	-0.2862
C	1.2984	3.4250	0.2537
C	1.7887	3.0669	1.6448
C	0.5702	4.7632	0.2569
H	2.1810	3.5238	-0.3957
H	2.3785	2.1502	1.6357
H	2.4146	3.8703	2.0361
H	0.9428	2.9343	2.3236
H	0.2127	5.0050	-0.7453
H	-0.2919	4.7143	0.9258
H	1.2290	5.5656	0.5925
H	0.2161	0.6238	-2.1699
H	0.5343	2.5969	-1.4720
C	0.7947	1.2852	-2.8642
O	0.8088	2.5255	-2.5348
O	1.2199	0.7635	-3.8584

Free Energy: -2229.4930968 hartrees

Compound J⁺



Cartesian Coordinates

Ru	0.7339	0.4232	-0.5430
N	1.3379	-1.6575	-0.7196
N	2.4317	-2.0399	-0.0341
N	1.2871	0.2447	1.4106
N	2.4009	-0.4441	1.7260
N	2.9100	0.7112	-0.9159
N	3.7412	-0.0697	-0.2063
C	3.2005	-1.0601	0.6952
H	4.0306	-1.5687	1.1765
C	0.9344	-2.7339	-1.3766
H	0.0597	-2.6870	-2.0047
C	1.7788	-3.8255	-1.1115
H	1.6985	-4.8255	-1.4973
C	2.7309	-3.3414	-0.2529

H	3.5853	-3.8032	0.2126
C	0.8022	0.7003	2.5538
H	-0.1098	1.2734	2.5616
C	1.6151	0.3040	3.6266
H	1.4745	0.5219	4.6696
C	2.6279	-0.4250	3.0595
H	3.4822	-0.9249	3.4835
C	3.6834	1.4477	-1.6928
H	3.2393	2.1704	-2.3577
C	5.0386	1.1379	-1.4852
H	5.8950	1.5735	-1.9673
C	5.0358	0.1575	-0.5261
H	5.8325	-0.3886	-0.0495
P	-1.4468	-0.0866	-0.1252
C	-1.7620	-0.9552	1.4537
C	-0.9275	-2.0184	1.8091
H	-0.1253	-2.3218	1.1477
C	-1.1158	-2.6952	3.0030
H	-0.4630	-3.5186	3.2621
C	-2.1352	-2.3107	3.8676
H	-2.2776	-2.8328	4.8048
C	-2.9682	-1.2572	3.5238
H	-3.7652	-0.9540	4.1901
C	-2.7870	-0.5839	2.3199
H	-3.4475	0.2349	2.0661

C	-2.0593	-1.2400	-1.3988
C	-2.6733	-2.4550	-1.1128
H	-2.8606	-2.7435	-0.0864
C	-3.0377	-3.3130	-2.1453
H	-3.5069	-4.2604	-1.9140
C	-2.7994	-2.9583	-3.4652
H	-3.0792	-3.6299	-4.2662
C	-2.2010	-1.7369	-3.7585
H	-2.0170	-1.4540	-4.7866
C	-1.8296	-0.8848	-2.7305
H	-1.3504	0.0609	-2.9630
C	-2.6929	1.2404	-0.1240
C	-2.4017	2.4114	0.5748
H	-1.4233	2.5366	1.0170
C	-3.3462	3.4220	0.6733
H	-3.1106	4.3272	1.2184
C	-4.5867	3.2761	0.0632
H	-5.3222	4.0670	0.1345
C	-4.8802	2.1162	-0.6406
H	-5.8443	1.9987	-1.1178
C	-3.9384	1.0984	-0.7317
H	-4.1814	0.1942	-1.2753
O	0.2920	2.3905	-0.7835
C	1.1564	3.4389	-0.4675
C	0.7091	4.1571	0.8055

C	1.2118	4.4222	-1.6333
H	2.1776	3.0723	-0.2860
H	0.6745	3.4592	1.6446
H	1.3953	4.9663	1.0651
H	-0.2884	4.5817	0.6655
H	1.5451	3.9199	-2.5433
H	0.2127	4.8259	-1.8174
H	1.8883	5.2540	-1.4254

Free Energy: -2039.722814 hartrees

Compound **[DBUH]⁺[HCOO]⁻**

Cartesian Coordinates

H	1.6323	0.9876	-0.2725
C	-0.2490	0.2552	-0.5138
C	0.1997	2.4290	0.4894
C	-1.2272	2.7651	0.0999
H	0.2909	2.3284	1.5733
C	-2.1128	1.5559	0.3382
H	-1.2665	3.0401	-0.9552
H	-3.1147	1.7257	-0.0526
C	0.2896	-1.0008	-1.1363
C	-2.4461	-0.7522	-0.5890
N	0.5996	1.1793	-0.1437
N	-1.5616	0.3888	-0.3520

H	0.8931	3.2035	0.1660
H	-1.5897	3.6083	0.6847
H	-2.1980	1.3396	1.4072
C	-2.3489	-1.7883	0.5304
C	0.0272	-2.2782	-0.2932
C	-0.8979	-2.0868	0.9096
H	-0.1559	-1.0896	-2.1281
H	1.3595	-0.8618	-1.2677
H	0.9928	-2.6256	0.0691
H	-0.3812	-3.0546	-0.9434
H	-0.5061	-1.2790	1.5356
H	-0.8684	-2.9849	1.5276
H	-2.1885	-1.2030	-1.5462
H	-3.4586	-0.3648	-0.6815
H	-2.8962	-1.4410	1.4089
H	-2.8425	-2.6984	0.1826
O	3.2220	0.7737	-0.4621
C	3.6189	-0.2510	0.1588
O	2.9276	-1.0557	0.7977
H	4.7137	-0.4374	0.1127

Free Energy: -651.622951 hartrees

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