

Electronic Supplementary Material (ESI) for Chemical Science.

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Disarming the Alkoxide Trap to Access a Practical FeCl₃ System for Borrowing Hydrogen *N*-alkylation

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1. General Information.

Unless otherwise noted, all manipulations were performed under a dry nitrogen atmosphere using Schlenk-line techniques or under a nitrogen atmosphere in the glovebox. All reagents obtained from commercially available sources were used without further purification unless otherwise stated. THF, diethyl ether, and toluene were obtained from commercial sources and were purified according to standard procedures. Reaction temperatures refer to external bath temperatures. TLC was performed on silica gel GF254 (layer thickness 0.20-0.25 mm) and components were located by observation under UV light. Column chromatography was performed on silica gel (300-400 mesh) using 10% ethyl acetate/hexane as eluent. NMR spectra were performed at room temperature on a Bruker Avance 400 spectrometer using the residual solvent signal as the internal standard [CDCl₃: 7.29 ppm (¹H), 77.00 ppm (¹³C). DMSO-*d*₆: 2.50 ppm (¹H), 39.52 ppm (¹³C)]R. GC analyses were recorded in a Shimadzu GC-2014C device equipped with a Wondacap 1 column. High-resolution mass spectra of compounds were recorded on LTQ Orbitrap Elite LC/MS (ESI) at the analytical center of Sun Yat-Sen University. UV-Vis spectroscopy data were obtained by use of a Hitachi U3500 at room temperature.

2. GC Analysis Method for the Condition Optimization and Control Experiments.

GC analysis method:

Injector: Mode: Split; temp.: 330 °C; Gas: N₂ Pressure: 1.34 bar; Split ratio: 39:1; Split flow: 67.6 mL/min. Column: Wondacap 1 column Capillary column (30 m × 0.25 mm); Nominal film thickness: 0.250 μm; Temperature program: Initial temperature 100 °C, heat to 120 °C with 5 °C/min, then heat to 200 °C with 50 °C/min, hold for 5 min. Initial Flow: 1.62 mL/min; Average velocity: 39.4 cm/sec, Pressure: 1.34 bar. Detector (FID): Temp.: 330 °C; Hydrogen flow: 40.0 mL/min; Air flow: 400.0 mL/min.

Preparation of GC sample:

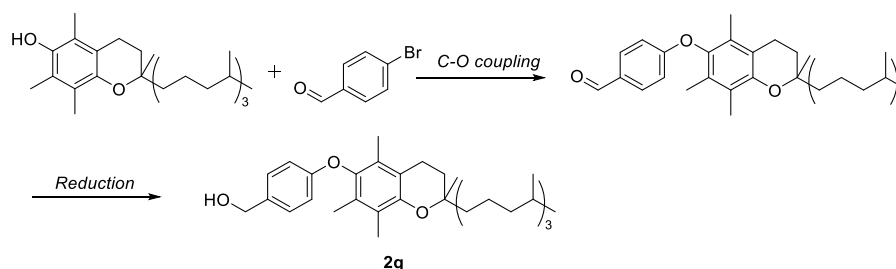
Dilute the crude reaction mixture with 10 mL of EtOAc and 21.0 mg (0.1 mmol) of 1,3,5-trimethoxybenzene was added as standard, filtered through the syringe filter, and collected in GC vials for analysis.

Retention times: Benzaldehyde: 2.79 min; Aniline: 2.83 min; Benzyl alcohol: 3.33 min; *N*-methylaniline: 3.62 min;

1,3,5-trimethoxybenzene: 6.55 min; *N*-1-diphenylmethanimine: 8.66 min; *N,N*-benzylphenylamine: 9.05 min.

3. Syntheses and Characterization of Substrates, Ligands, and Catalysts.

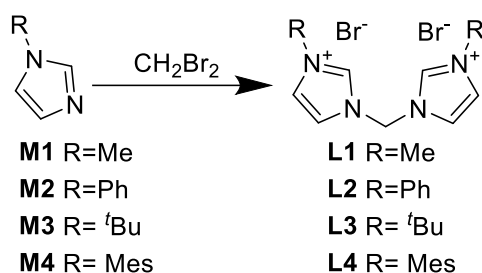
Scheme S1. Synthesis of the vitamin E, (±)- α -tocopherol, a derivative of 4-bromobenzyl alcohol (2q)¹



(4-((R)-2,5,7,8-Tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yloxy) phenyl)methanol.¹ 4-Bromobenzaldehyde (4 mmol, 740 mg), Pd(OAc)₂ (4 mol%, 0.16 mmol, 36 mg), JhonPhos (6 mol%, 0.24 mmol, 70 mg), K₃PO₄ (2.17 equiv, 8.67 mmol, 1.84 g) were taken in an oven-dried Schlenk reaction tube, charged with magnetic stir bar. Then the reaction tube was evacuated and back filled with nitrogen. This vacuum/ nitrogen sequence was repeated four times, (R)-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-ol (vitamin E) (4 mmol, 1.72 g), Toluene (4 mL) were added under the positive pressure of nitrogen and the resealed tube

was immersed in a preheated oil bath at 120 °C and stirred vigorously for 24 hours. The reaction mixture was cooled to room temperature, diluted with 10 mL ethyl acetate, and filtered through celite using additional 20 mL ethyl acetate. The filtrate was concentrated and purified by column chromatography eluting with pet ether - ethyl acetate mixture (99:1 v/v) to give the product aldehyde. The aldehyde was taken in a clean round bottom flask, charged with a magnetic stir bar. Ethanol was added to dissolve the aldehyde and placed on a magnetic stirrer. NaBH₄ (1.5 equiv) was added to this solution in portion-wise with constant stirring at room temperature. The reaction mixture was stirred at room temperature for complete conversion (checking by TLC). The remaining ethanol was removed in rota-vap. Then water was added to this reaction mixture and the organic part was extracted by diethyl ether and dried over anhydrous Na₂SO₄. Organic part was concentrated and brown coloured liquid(4-((R)-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yloxy) phenyl)methanol was isolated through silica gel, eluted with pet ether - ethyl acetate mixture (8:1 v/v). ¹H NMR (400 MHz, CDCl₃) δ 7.30 - 7.22 (m, 2H), 6.82 - 6.72 (m, 2H), 4.60 (s, 2H), 2.66 (t, *J* = 6.5 Hz, 2H), 2.18 (s, 3H), 2.06 (s, 3H), 2.02 (s, 3H), 1.88 (ddq, *J* = 19.8, 13.2, 6.7 Hz, 2H), 1.70 - 1.53 (m, 4H), 1.53 - 1.41 (m, 4H), 1.41 - 1.27 (m, 10H), 1.25 - 1.12 (m, 6H), 0.93 (t, *J* = 6.5 Hz, 12H); HRMS (ESI⁺, MeOH) [M + Na]⁺ 559.41228.

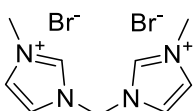
Scheme S2. Synthesis of the Imidazolium Salts L1–L4



General Method for the Preparation of Imidazolium Salts L1-L4.^{2,3}

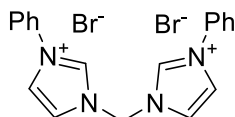
To a solution of the *N*-substituted imidazole (20 mmol) in 5 mL of THF in a sealed tube (15 mL) was added dibromomethane (10 mmol). The mixture is stirred at 130 °C for 2-3 days, and the solid that precipitates is filtered and washed repeatedly with an excess amount of THF and CH₂Cl₂. The white solid was dried in vacuo, and **L1-L4** are obtained.

Synthesis of 1,1-Bis(3-methylimidazolium-1-yl)methane dibromide (L1)²



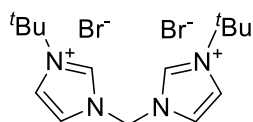
Following the general method (2 days) using 1-methylimidazole (1.59 mL, 20 mmol) and dibromomethane (0.7 mL, 10 mmol) in 5 mL of THF, gave **L1** as a white solid. Yield: 2.84 g (8.40 mmol, 85%). ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.58 (s, 2H), 8.11 (t, *J* = 1.8 Hz, 2H), 7.83 (t, *J* = 1.7 Hz, 2H), 6.79 (s, 2H), 3.91 (s, 6H); ¹³C NMR (101 MHz, DMSO-*d*₆) δ 138.01, 124.26, 121.89, 57.79, 36.24; MS (ESI⁺, MeOH) [(M - 2Br)]²⁺ 88.95.

Synthesis of 1,1-Bis(3-phenylimidazolium-1-yl)methane dibromide (L2)²



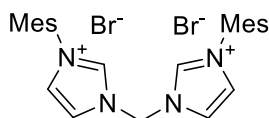
Following the general method (2 days) using 1-phenylimidazole (2.88 g, 20 mmol) and dibromomethane (0.7 mL, 10mmol) in 5 mL of THF, gave **L2** as a white solid. Yield: 2.58 g (5.58 mmol, 56%). ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.47 (s, 2H), 8.48 (s, 4H), 7.85 (d, *J* = 7.8 Hz, 4H), 7.71 (t, *J* = 7.6 Hz, 4H), 7.63 (t, *J* = 7.3 Hz, 2H), 6.98 (s, 2H); ¹³C NMR (101 MHz, DMSO-*d*₆) δ 137.33, 134.45, 130.27, 130.18, 123.03, 121.92, 121.52, 58.31; MS (ESI⁺, MeOH) [(M - 2Br)]²⁺ 150.95.

Synthesis of 1,1-Bis(3-*tert*-butylimidazolium-1-yl)methane dibromide (**L3**)³



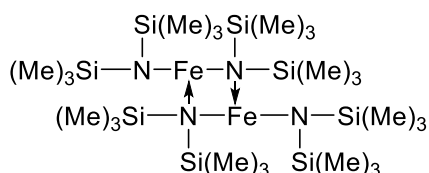
Following the general method (3 days) using 1-*tert*-butylimidazole (2.48 g, 20 mmol) and dibromomethane (0.7 mL, 10 mmol) in 5 mL of THF, gave **L3** as a white solid. Yield: 2.65 g (6.28 mmol, 63%). ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.87 (s, 2 H), 8.24 (s, 2 H), 8.18 (s, 2 H), 6.69 (s, 2 H), 1.63 (s, 18 H); MS (ESI⁺, MeOH) [(M - 2Br)]²⁺ 130.99.

Synthesis of 1,1-Bis(3-mesitylimidazolium-1-yl)methane dibromide (**L4**)³



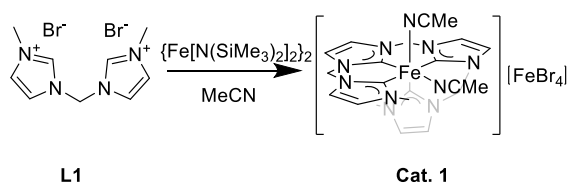
Following the general method (3 days) using 1-mesitylimidazole (3.73 g, 20 mmol) and dibromomethane (0.7 mL, 10 mmol) in 5 mL of THF, gave **L4** as a white solid. Yield: 3.74 g (6.85 mmol, 68%). ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.56 (s, 2 H), 8.96 (d, 2 H), 8.54 (d, 2 H), 7.61 (s, 4 H), 7.41 (s, 2 H), 3.79 (d, 6 H), 2.78 (s, 6 H), 2.49 (s, 6 H); MS (ESI⁺, MeOH) [(M - 2Br)]²⁺ 193.01.

Synthesis of {Fe[N(SiMe₃)₂]₂}⁴



A flame-dried Schlenk-flask was charged with LiN(SiMe₃)₂ (6.54 g, 2.2 equiv, 38.2 mmol) in diethyl ether (60 mL) in a glove box full of nitrogen. FeCl₂ (2.25 g, 1.0 equiv, 17.2 mmol) previously charged full of argon in a flame-dried Schlenk was added in portions at 0 °C. The resulting reaction mixture was allowed to warm to room temperature and stirred for 24 h. The Et₂O was removed under vacuum, then the solid residue was suspended in *n*-hexane (25 mL) filtered over a glass frit, and washed with *n*-hexane (5 × 3 mL). After removing the solvent under reduced pressure, the crude product was purified by distillation under reduced pressure to obtain a dark green oil that crystallizes upon standing at room temperature. Yield: 2.20 g (2.92 mmol, 34%). ¹H NMR (400 MHz, C₆D₆) δ 64.71 (bs).

Scheme S3. Synthesis of Cat. 1

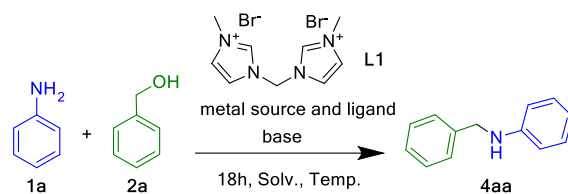


Synthesis of tetracarbeno iron(II) complex (Cat.1)⁵

A suspension of the imidazolium salt **L1** (225.4 mg, 0.667 mmol) in MeCN (5 mL) was treated with {Fe[N(SiMe₃)₂]₂} (314 mg, 0.417 mmol) and stirred overnight at room temperature. The precipitate was filtered off and washed with THF (2 mL) and Et₂O (2 mL). The desired complex was obtained as a yellow powder (232.4 mg, 0.267 mmol, 40%) upon drying under vacuum. NMR measurements were hampered by the paramagnetic tetrabromoferrate(II), though the tetracarbeno complex itself is diamagnetic.⁵ HRMS (ESI⁺, MeCN): [M - FeBr₃ - 2MeCN]⁺ 487.0656, [L₂Fe]²⁺ 204.0736. Anal. Calcd for **Cat.1** (C₂₂H₃₀Br₄Fe₂N₁₀): C, 30.52; H, 3.49; N, 16.18, Calcd for 1 **Cat.1** + 1.329 CH₃CN: C, 32.18; H, 3.72; N, 17.24, Calcd for 1 **Cat.1** + 0.818 CH₃CN + 0.187 HN(SiMe₃)₂: C, 31.99; H, 3.90; N, 16.58. Found: C, 32.14; H, 3.90; N, 16.53.

4. Optimization of Reaction Conditions.

Table S1. Optimization of Reaction Conditions for Amination of Benzyl Alcohol (2a) with Aniline (1a)^a



Entry	T/°C (time)	Ligand	metal source	solvent	base	yeild ^b /%
1	80	L1 7.2 mol%	Cr(CO) ₆ 3.0 mol%	toluene	^t BuOK 1.2 equiv	<5
2	110	L1 7.2 mol%	MnCl ₂ 1.5 mol% + Mn 1.5 mol%	toluene	^t BuOK 1.2 equiv	42
3	80	L1 7.2 mol%	FeCl ₂ 3.0 mol%	toluene	^t BuOK 1.2 equiv	65
4	80	L1 7.2 mol%	Co(NH ₃) ₆ Cl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	9
5	80	none	none	toluene	^t BuOK 1.2 equiv	<5
6	110	L1 7.2 mol%	FeCl ₂ 3.0 mol%	toluene	^t BuOK 1.2 equiv	84
7	110	L1 7.2 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	92
8	110	L1 3.6 mol%	Fe(Cp) ₂ 3.0 mol%	toluene	^t BuOK 1.2 equiv	20
9	110	L1 3.6 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	65
10	110	L1 3.6 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuONa 1.2 equiv	13
11	110	L1 3.6 mol%	FeCl ₃ 3.0 mol%	toluene	CsCO ₃ 1.2 equiv	<5
12	110	L1 3.6 mol%	FeCl ₃ 3.0 mol%	toluene	KOH 1.2 equiv	23
13	110	L1 3.6 mol%	FeCl ₃ 3.0 mol%	toluene	NaOH 1.2 equiv	6
14	110	L1 3.6 mol%	FeCl ₃ 3.0 mol%	toluene	none	trace
15	110	L1 1.5 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	41
16	110	L1 3.0 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	64
17	110	L1 4.5 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	68

18	110	L1 6.0 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	75
19	110	L1 7.5 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	91
20	110	L1 9.0 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	88
21	RT (7 day)	L1 7.2 mol%	FeCl ₃ 3.0 mol%	toluene	^t BuOK 1.2 equiv	41
22	110	L1 7.2 mol%	FeCl ₃ 3.0 mol%	H ₂ O	^t BuOK 1.2 equiv	trace
23	110	L1 7.2 mol%	FeCl ₃ 3.0 mol%	MeCN	^t BuOK 1.2 equiv	<5
24	110	L1 7.2 mol%	FeCl ₃ 3.0 mol%	DMSO	^t BuOK 1.2 equiv	trace
25	110	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.2 equiv	>99
26	80	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.2 equiv	>99
27	60	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.2 equiv	74
28	40	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.2 equiv	17
29	80	L1 4.8 mol%	FeCl ₃ 2.0 mol%	THF	^t BuOK 1.2 equiv	98
30	80	L1 4.8 mol%	FeCl ₂ 2.0 mol%	THF	^t BuOK 1.2 equiv	99
31	80	L1 2.4 mol%	FeCl ₃ 1.0 mol%	THF	^t BuOK 1.2 equiv	65
32	80	L1 2.4 mol%	FeCl ₂ 1.0 mol%	THF	^t BuOK 1.2 equiv	84
33	80	L1 1.2 mol%	FeCl ₃ 0.5 mol%	THF	^t BuOK 1.2 equiv	15
34	80	L1 1.2 mol%	FeCl ₂ 0.5 mol%	THF	^t BuOK 1.2 equiv	63
35	80	L1 1.2 mol%	Fe 3.0 mol%	THF	^t BuOK 1.2 equiv	<5
36	80	L1 1.2 mol%	FeCl ₃ 1.0 mol% + Fe 1.0 mol%	THF	^t BuOK 1.2 equiv	90
37	80	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.0 equiv	70
38	80	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.6 equiv	97
39	80	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 2.0 equiv	93

40	80	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 2.4 equiv	75
41	80 (6 h)	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.2 equiv	69
42	80 (12 h)	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.2 equiv	92
43	80 (24 h)	L1 7.2 mol%	FeCl ₃ 3.0 mol%	THF	^t BuOK 1.2 equiv	>99

^aGeneral reaction conditions: 1a (0.5 mmol, 1 equiv), 2a (0.6 mmol), 1mL of solvent, dry nitrogen atmosphere.

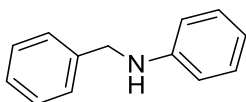
^bYield was determined by GC analysis with FID.

5. General Procedure for the *in-situ* Catalytic *N*-alkylation of Amines with Alcohols.

In a glovebox, FeCl₃ (3.0 mol%), 1,1'-dimethyl-3,3'-methylenediimidazolium dibromide (**L1**, 7.2 mol%) ^tBuOK (0.6 mmol), amine (0.5 mmol) and alcohol (0.6 mmol) were mixed with THF (1.0 mL) in a 15 mL flame-dried Schlenk tube equipped with a magnetic stirring bar and a Teflon cap. After, the sealed reaction tube was brought outside the glovebox. The mixture was then stirred at 80 °C for 18 h. After completion of the reaction, the reaction mixture was cooled to ambient temperature and 5 mL of water was added and the aqueous solution was extracted with CH₂Cl₂ (3 × 5 mL). The combined extracts were dried over anhydrous Na₂SO₄, the solvent removed and the crude product purified on a flash chromatography column.

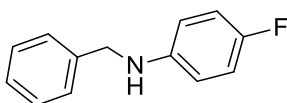
6. Analytical Data of *N*-alkylated Anilines.

N-benzylaniline (**4aa**).²



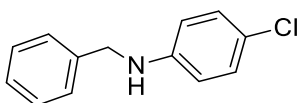
The compound was prepared as described in the general method (colorless oil, 98% isolated yield, 90.2 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.47 – 7.41 (m, 4H), 7.39 – 7.33 (m, 1H), 7.29 – 7.23 (m, 2H), 6.81 (t, *J* = 6.5 Hz, 1H), 6.71 (d, *J* = 7.8 Hz, 2H), 4.39 (s, 2H), 4.08 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 183.65.

N-benzyl-4-fluoroaniline (**4ba**).²



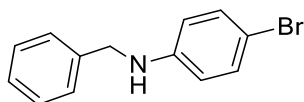
The compound was prepared as described in the general method (colorless oil, 89% isolated yield, 89.4 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.43 – 7.36 (m, 4H), 7.36 – 7.30 (m, 1H), 6.93 (t, *J* = 8.7 Hz, 2H), 6.65 – 6.54 (m, 2H), 4.32 (s, 2H), 3.94 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 201.60.

N-benzyl-4-chloroaniline (**4ca**).²



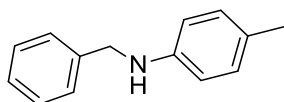
The compound was prepared as described in the general method (colorless oil, 91% isolated yield, 99.5 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.36 (d, *J* = 4.3 Hz, 4H), 7.33 – 7.27 (m, 1H), 7.12 (d, *J* = 8.6 Hz, 2H), 6.56 (d, *J* = 8.6 Hz, 2H), 4.31 (s, 2H), 4.08 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 217.60.

N-benzyl-4-bromoaniline (**4da**).²



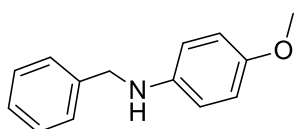
The compound was prepared as described in the general method (colorless oil, 94% isolated yield, 123.8 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.36 – 7.32 (m, 4H), 7.32 – 7.27 (m, 1H), 7.24 (d, *J* = 8.7 Hz, 2H), 6.49 (d, *J* = 8.8 Hz, 2H), 4.28 (s, 2H), 4.05 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 263.40.

N-benzyl-4-methylaniline (**4ea**).²



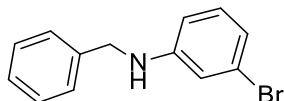
The compound was prepared as described in the general method (colorless oil, 81% isolated yield, 80.1 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.43 – 7.37 (m, 4H), 7.34 – 7.28 (m, 1H), 7.03 (d, *J* = 8.3 Hz, 2H), 6.61 (d, *J* = 8.4 Hz, 2H), 4.35 (s, 2H), 3.94 (s, 1H), 2.29 (s, 3H); MS (ESI⁺, MeOH) [M + H]⁺ 198.65.

N-benzyl-4-methoxyaniline (**4fa**).²



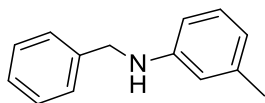
The compound was prepared as described in the general method (colorless oil, 63% isolated yield, 67.0 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.36 (m, 4H), 7.30 – 7.27 (m, 1H), 6.80 (d, *J* = 8.0 Hz, 2H), 6.63 (d, *J* = 8.0 Hz, 2H), 4.31 (s, 2H), 3.86 (s, 1H), 3.77 (s, 3H); MS (ESI⁺, MeOH) [M + H]⁺ 213.60.

N-benzyl-3-bromoaniline (**4ga**).²



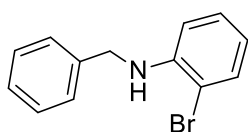
The compound was prepared as described in the general method (colorless oil, 84% isolated yield, 110.3 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.37 – 7.34 (m, 4H), 7.32 – 7.29 (m, 1H), 7.01 (t, *J* = 8.0 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 6.79 (s, 1H), 6.54 (d, *J* = 7.9 Hz, 1H), 4.31 (d, *J* = 5.1 Hz, 2H), 4.11 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 263.40.

N-benzyl-3-methylaniline (**4ha**).²



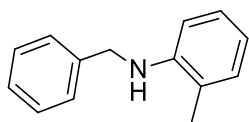
The compound was prepared as described in the general method (colorless oil, 82% isolated yield, 81.3 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.38 (d, *J* = 7.6 Hz, 4H), 7.33 – 7.26 (m, 1H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.57 (d, *J* = 7.1 Hz, 1H), 6.48 (d, *J* = 13.5 Hz, 2H), 4.34 (s, 2H), 3.98 (s, 1H), 2.30 (s, 3H); MS (ESI⁺, MeOH) [M + H]⁺ 198.65.

N-benzyl-2-bromoaniline (**4ia**).²



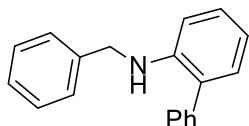
The compound was prepared as described in the general method (colorless oil, 87% isolated yield, 114.5 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.51 (d, *J* = 7.8 Hz, 1H), 7.44 – 7.40 (m, 4H), 7.37 – 7.32 (m, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 6.69 – 6.60 (m, 2H), 4.83 (s, 1H), 4.45 (d, *J* = 4.9 Hz, 2H); MS (ESI⁺, MeOH) [M + H]⁺ 263.40.

N-benzyl-2-methylaniline (**4ja**).²



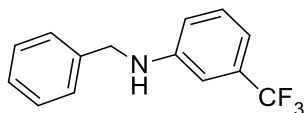
The compound was prepared as described in the general method (colorless oil, 64% isolated yield, 62.9 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.47 – 7.36 (m, 4H), 7.33 (t, *J* = 6.5 Hz, 1H), 7.19 – 7.07 (m, 2H), 6.72 (t, *J* = 7.4 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 4.41 (s, 2H), 3.90 (s, 1H), 2.21 (s, 3H); MS (ESI⁺, MeOH) [M + H]⁺ 198.56.

N-benzyl-[1,1'-biphenyl]-2-amine (**4ka**).²



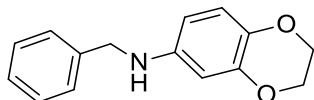
The compound was prepared as described in the general method (colorless oil, 77% isolated yield, 99.5 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.56 – 7.45 (m, 4H), 7.40 – 7.34 (m, 5H), 7.32 – 7.28 (m, 1H), 7.26 – 7.21 (m, 1H), 7.17 (d, *J* = 7.2 Hz, 1H), 6.83 (t, *J* = 7.4 Hz, 1H), 6.71 (d, *J* = 8.2 Hz, 1H), 4.42 (s, 1H), 4.37 (s, 2H); MS (ESI⁺, MeOH) [M + H]⁺ 259.95.

N-Benzyl-3-(trifluoromethyl)aniline (**4ma**).¹



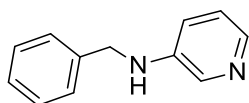
The compound was prepared as described in the general method (colorless oil, 74% isolated yield, 93.1 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.39 (m, 4H), 7.36 – 7.31 (m, 1H), 7.27 (t, *J* = 7.9 Hz, 1H), 6.99 – 6.96 (m, 1H), 6.87 (s, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 4.38 (s, 2H), 4.24 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 252.57.

N-benzyl-2,3-dihydrobenzo[*b*][1,4]dioxin-6-amine (**4na**).²



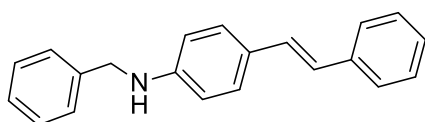
The compound was prepared as described in the general method (yellow oil, 81% isolated yield, 98.1 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.32 (m, 4H), 7.31 – 7.26 (m, 1H), 6.72 (d, *J* = 8.4 Hz, 1H), 6.24 – 6.17 (m, 2H), 4.26 (s, 2H), 4.24 – 4.21 (m, 2H), 4.20 – 4.16 (m, 2H), 3.42 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 241.87.

N-benzylpyridin-3-amine (**4oa**).²



The compound was prepared as described in the general method (yellow oil, 91% isolated yield, 84.1 mg). ¹H NMR (400 MHz, CDCl₃) δ 8.06 (s, 1H), 8.01 – 7.91 (m, 1H), 7.40 – 7.31 (m, 4H), 7.31 – 7.25 (m, 1H), 7.08 – 7.02 (m, 1H), 6.86 (d, *J* = 7.9 Hz, 1H), 4.33 (s, 2H), 4.25 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 184.88.

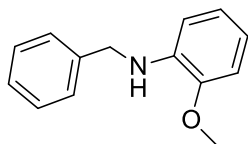
(*E*)-*N*-benzyl-4-styrylaniline (**4ra**).²



The compound was prepared as described in the general method (white solid, 99% isolated yield, 142.0 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.53 – 7.48 (m, 2H), 7.42 – 7.32 (m, 9H), 7.24 (t, *J* = 6.4 Hz, 1H), 7.11 – 6.91 (m, 2H), 6.70 – 6.61 (m, 2H), 4.38 (s, 2H), 4.17 (q, *J* = 7.1 Hz,

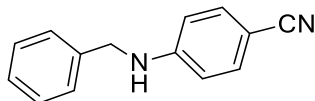
1H); MS (ESI⁺, MeOH) [M + H]⁺ 285.90.

N-benzyl-2-methoxyaniline (**4ta**).⁶



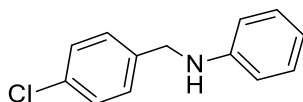
The compound was prepared as described in the general method (colorless oil, 76% isolated yield, 80.6 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.39 (m, 3H), 7.37 – 7.35 (m, 2H), 7.35 – 7.33 (m, 1H), 6.85 (td, *J* = 7.6, 1.3 Hz, 1H), 6.81 (dd, *J* = 7.9, 1.2 Hz, 1H), 6.70 (td, *J* = 7.7, 1.5 Hz, 1H), 6.62 (dd, *J* = 7.8, 1.4 Hz, 1H), 4.65 (s, 1H), 4.37 (s, 2H), 3.86 (s, 3H); MS (ESI⁺, MeOH) [M + H]⁺ 214.40.

4-(Benzylamino)benzonitrile (**4ua**).⁷



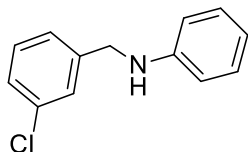
The compound was prepared as described in the general method (yellow oil, 88% isolated yield, 83.7 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.45 – 7.27 (m, 7H), 6.59 (d, *J* = 8.8 Hz, 2H), 4.74 (s, 1H), 4.38 (d, *J* = 5.6 Hz, 2H); MS (ESI⁺, MeOH) [M + H]⁺ 209.48.

N-(4-chlorobenzyl)aniline (**4ab**).²



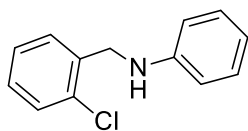
The compound was prepared as described in the general method (yellow oil, 82% isolated yield, 89.4 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.36 – 7.30 (m, 4H), 7.25 – 7.18 (m, 2H), 6.77 (t, *J* = 7.3 Hz, 1H), 6.67 – 6.60 (m, 2H), 4.33 (s, 2H), 4.07 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 218.50.

N-(3-chlorobenzyl)aniline (**4ac**).²



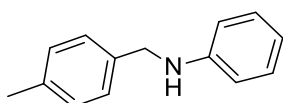
The compound was prepared as described in the general method (yellow oil, 85% isolated yield, 92.4 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.42 (s, 1H), 7.34 – 7.28 (m, 3H), 7.28 – 7.20 (m, 2H), 6.80 (t, *J* = 6.8 Hz, 1H), 6.66 (d, *J* = 7.8 Hz, 2H), 4.34 (s, 2H), 4.10 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 218.56.

N-(2-chlorobenzyl)aniline (**4ad**).⁸



The compound was prepared as described in the general method (orange oil, 50% isolated yield, 54.8 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.28 – 7.26 (m, 2H), 7.26 – 7.13 (m, 4H), 6.72 (t, *J* = 7.3 Hz, 1H), 6.63 (t, *J* = 8.7 Hz, 2H), 4.38 (d, *J* = 42.8 Hz, 2H), 4.12 (s, 1H); MS (ESI⁺, MeOH) [M + H]⁺ 218.65.

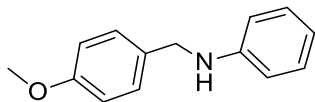
N-(4-methylbenzyl)aniline (**4ae**).²



The compound was prepared as described in the general method (yellow oil, 99% isolated yield, 97.3 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.31 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.18 (m, 4H), 6.76 (tt, *J* = 7.3, 1.1 Hz, 1H), 6.72 – 6.65 (m, 2H), 4.32 (s, 2H), 4.01 (s, 1H), 2.40 (s, 3H); MS (ESI⁺,

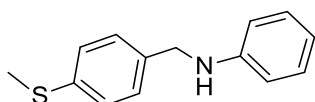
MeOH) $[M + H]^+$ 198.65.

N-(4-methoxybenzyl)aniline (**4af**).²



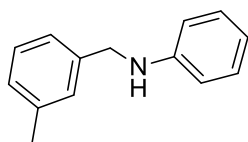
The compound was prepared as described in the general method (yellow oil, 98% isolated yield, 104.6 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.34 (d, J = 8.6 Hz, 2H), 7.23 (ddd, J = 8.4, 5.7, 1.9 Hz, 2H), 6.93 (d, J = 8.6 Hz, 2H), 6.77 (t, J = 7.3 Hz, 1H), 6.68 (d, J = 7.7 Hz, 2H), 4.29 (s, 2H), 3.99 (s, 1H), 3.84 (s, 3H); MS (ESI⁺, MeOH) $[M + H]^+$ 214.60.

N-(4-(methylthio)benzyl)aniline (**4ag**).²



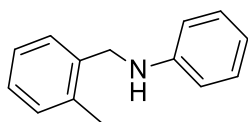
The compound was prepared as described in the general method (yellow oil, 90% isolated yield, 102.3 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.36 – 7.24 (m, 4H), 7.24 – 7.16 (m, 2H), 6.79 – 6.71 (m, 1H), 6.66 (d, J = 7.8 Hz, 2H), 4.31 (s, 2H), 4.04 (s, 1H), 2.51 (s, 3H); MS (ESI⁺, MeOH) $[M + H]^+$ 230.90.

N-(3-methylbenzyl)aniline (**4ah**).²



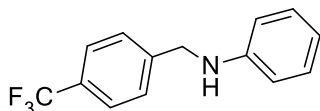
The compound was prepared as described in the general method (yellow oil, 86% isolated yield, 85.0 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.26 (m, 5H), 7.22 (d, J = 7.3 Hz, 1H), 6.85 (t, J = 7.3 Hz, 1H), 6.76 (d, J = 8.1 Hz, 2H), 4.39 (s, 2H), 4.08 (s, 1H), 2.48 (s, 3H); MS (ESI⁺, MeOH) $[M + H]^+$ 198.68.

N-(2-methylbenzyl)aniline (**4ai**).²



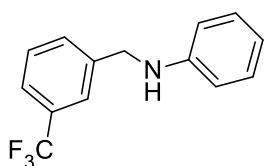
The compound was prepared as described in the general method (yellow oil, 86% isolated yield, 84.8 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.37 (d, J = 7.3 Hz, 1H), 7.25 – 7.21 (m, 5H), 6.76 (t, J = 7.3 Hz, 1H), 6.67 (d, J = 7.9 Hz, 2H), 4.30 (s, 2H), 3.86 (s, 1H), 2.41 (s, 3H); MS (ESI⁺, MeOH) $[M + H]^+$ 198.62.

N-(4-(trifluoromethyl)benzyl)aniline (**4aj**).⁹



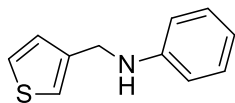
The compound was prepared as described in the general method (yellow oil, 46% isolated yield, 57.9 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.65 – 7.59 (m, 2H), 7.49 (d, J = 7.9 Hz, 2H), 7.18 (t, J = 7.8 Hz, 2H), 6.74 (t, J = 7.3 Hz, 1H), 6.61 (d, J = 8.0 Hz, 2H), 4.42 (s, 2H), 4.15 (s, 1H); MS (ESI⁺, MeOH) $[M + H]^+$ 252.65.

N-(3-(trifluoromethyl)benzyl)aniline (**4ak**).²



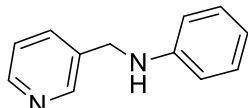
The compound was prepared as described in the general method (yellow oil, 75% isolated yield, 94.0 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.71 (s, 1H), 7.62 (t, $J = 8.1$ Hz, 2H), 7.51 (t, $J = 7.7$ Hz, 1H), 7.30 – 7.21 (m, 2H), 6.82 (t, $J = 7.3$ Hz, 1H), 6.69 (d, $J = 7.8$ Hz, 2H), 4.45 (s, 2H), 4.15 (s, 1H); MS (ESI $^+$, MeOH) $[\text{M} + \text{Na}]^+$ 274.03.

N-(thiophen-3-ylmethyl)aniline (**4al**).²



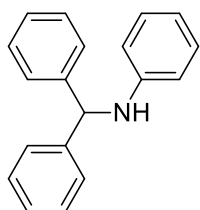
The compound was prepared as described in the general method (yellow oil, 82% isolated yield, 77.8 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.36 – 7.31 (m, 1H), 7.26 – 7.17 (m, 3H), 7.15 – 7.08 (m, 1H), 6.77 (t, $J = 7.3$ Hz, 1H), 6.68 (d, $J = 7.7$ Hz, 2H), 4.36 (s, 2H), 3.99 (s, 1H); MS (ESI $^+$, MeOH) $[\text{M} + \text{H}]^+$ 189.75.

N-(pyridin-3-ylmethyl)aniline (**4am**).²



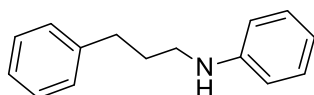
The compound was prepared as described in the general method (yellow oil, 90% isolated yield, 82.4 mg). ^1H NMR (400 MHz, CDCl_3) δ 8.62 (s, 1H), 8.51 (d, $J = 3.8$ Hz, 1H), 7.69 (d, $J = 7.8$ Hz, 1H), 7.30 – 7.22 (m, 1H), 7.22 – 7.12 (m, 2H), 6.74 (t, $J = 7.3$ Hz, 1H), 6.66 – 6.57 (m, 2H), 4.35 (s, 2H), 4.25 – 3.83 (m, 1H); MS (ESI $^+$, MeOH) $[\text{M} + \text{H}]^+$ 184.81.

N-Benzhydrylaniline (**4an**).¹⁰



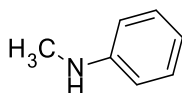
The compound was prepared as described in the general method at 90 °C (yellow liquid, 51% isolated yield, 66.4 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.37 – 7.16 (m, 12H), 6.79 – 6.77 (m, 1H), 6.77 – 6.65 (m, 2H), 5.78 (s, 1H), 3.11 (s, 1H); MS (ESI $^+$, MeOH) $[\text{M} + \text{H}]^+$ 258.64.

N-(3-phenylpropyl)aniline (**4ao**).²



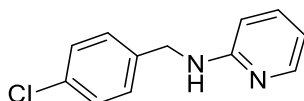
The compound was prepared as described in the general method (yellow oil, 69% isolated yield, 73.0 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.42 (d, $J = 6.8$ Hz, 1H), 7.36 – 7.21 (m, 6H), 6.81 (t, $J = 6.8$ Hz, 1H), 6.72 (d, $J = 8.2$ Hz, 2H), 4.34 (s, 2H), 3.91 (s, 1H), 2.50 – 2.37 (m, 4H); MS (ESI $^+$, MeOH) $[\text{M} + \text{H}]^+$ 211.60.

N-methylaniline (**4ap**).⁸



The compound was prepared as described in the general method (yellow liquid, 60% isolated yield, 32.1 mg). ^1H NMR (400 MHz, CDCl_3) δ 7.21 (t, $J = 7.9$ Hz, 2H), 6.73 (t, $J = 7.3$ Hz, 1H), 6.64 (d, $J = 7.9$ Hz, 2H), 3.70 (s, 1H), 2.85 (s, 3H); MS (ESI $^+$, MeOH) $[\text{M} + \text{H}]^+$ 108.65.

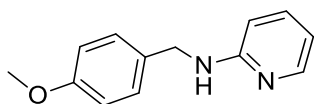
N-(4-Chlorobenzyl)pyridin-2-amine (**4sb**).¹



The compound was prepared as described in the general method (white solid, 99% isolated yield, 108.0 mg). ^1H NMR (400 MHz, CDCl_3) δ

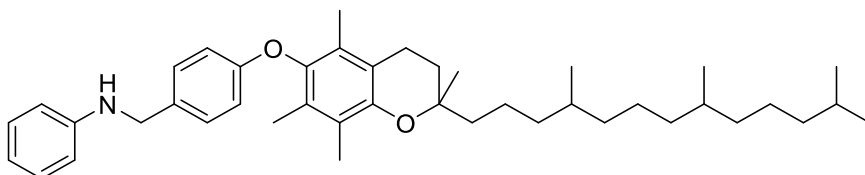
8.09 (d, $J = 4.2$ Hz, 1H), 7.39 (t, $J = 8.6$ Hz, 1H), 7.29 (s, 4H), 6.63 – 6.57 (m, 1H), 6.34 (d, $J = 8.4$ Hz, 1H), 5.02 (s, 1H), 4.48 (d, $J = 6.0$ Hz, 2H); MS (ESI⁺, MeOH) [M + H]⁺ 219.1.

N-(4-Methoxybenzyl)pyridin-2-amine (**4sf**).¹



The compound was prepared as described in the general method (white solid, 99% isolated yield, 106.8 mg). ¹H NMR (400 MHz, CDCl₃) δ 8.09 (d, $J = 4.8$ Hz, 1H), 7.39 (t, $J = 6.9$ Hz, 1H), 7.28 (d, $J = 8.6$ Hz, 2H), 6.87 (d, $J = 8.6$ Hz, 2H), 6.62 – 6.54 (m, 1H), 6.36 (d, $J = 8.4$ Hz, 1H), 4.90 (s, 1H), 4.42 (d, $J = 5.6$ Hz, 2H), 3.79 (s, 3H); MS (ESI⁺, MeOH) [M + H]⁺ 215.1.

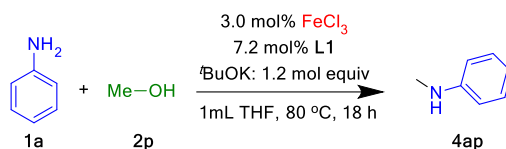
N-(4-Methoxybenzyl)pyridin-2-amine (**4aq**).



The compound was prepared as described in the general method (white solid, 66% isolated yield, 201.9 mg). ¹H NMR (400 MHz, CDCl₃) δ 7.23 (d, $J = 8.4$ Hz, 2H), 6.75 (d, $J = 8.4$ Hz, 2H), 4.58 (s, 2H), 2.65 (d, $J = 6.5$ Hz, 2H), 2.16 (s, 3H), 2.04 (s, 3H), 2.00 (s, 3H), 1.86 (ddq, $J = 19.8, 13.2, 6.7$ Hz, 2H), 1.31 (s, 24H), 0.91 (t, $J = 6.5$ Hz, 12H); ¹³C NMR (101 MHz, CDCl₃) δ 158.29, 148.85, 148.36, 143.54, 132.24, 131.65, 129.33, 129.06, 128.28, 126.34, 123.38, 117.95, 117.57, 114.92, 112.90, 75.11, 47.98, 40.14, 39.52, 37.61, 37.55, 37.44, 37.43, 32.83, 31.45, 28.11, 24.95, 24.59, 23.98, 22.87, 22.78, 21.16, 20.76, 19.91, 19.84, 19.83, 13.04, 12.16, 11.96; HRMS (ESI⁺, MeOH) [M + H]⁺ 612.47050.

7. *N*-methylation of Aniline with Methanol.

Table S2. *N*-methylation for Amination of Methanol (2p) with Aniline (1a)^a



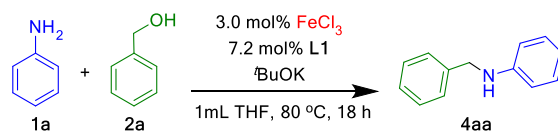
Entry	T/°C (time)	solvent	base	yield ^b /%
1	80	THF	^t BuOK 1.2 equiv	21
2	80	MeOH	^t BuOK 1.2 equiv	trace
3	60	THF	^t BuOK 1.2 equiv	26
4	40	THF	^t BuOK 1.2 equiv	7
5	80	THF	^t BuOK 1.2 equiv	<5

^aGeneral reaction conditions: 1a (0.5 mmol, 1 equiv), 2a (0.6 mmol), 1mL of solvent, dry nitrogen atmosphere.

^bYield was determined by GC analysis with FID and 1,3,5-trimethoxybenzene as standard.

8. *N*-alkylation of Amines with Different amount of Alcohols and Base

Table S3. Amination of Different Amount of Benzyl Alcohol (2a) and ^tBuOK with Aniline (1a)^a



Entry	T/°C (time)	solvent	Benzyl Alcohol	base	yeild ^b /%
1	80	THF	1.2 equiv	^t BuOK 1.2 equiv	>99
2	80	THF	4.0 equiv	^t BuOK 1.2 equiv	33
3	80	THF	4.0 equiv	^t BuOK 4.0 equiv	97
4 ^c	80	THF	4.0 equiv	^t BuOK 1.2 equiv	49
5	80	THF	1 mL ^d	^t BuOK 1.2 equiv	trace

^aGeneral reaction conditions: 1a (0.5 mmol, 1 equiv), 1mL of solvent, dry nitrogen atmosphere.

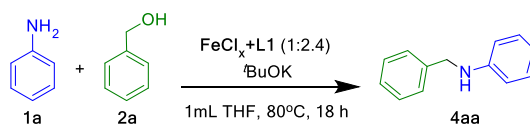
^bYield was determined by GC analysis with FID.

^cA3 molecular sieve was added.

^dUse benzyl alcohol as solvent instead of THF.

9. Detection of the Reduction of Iron(III).

Table S4. Hydrogen produce by Amination of Benzyl Alcohol (1a) with Aniline (2a)^a



entry	FeCl _x	^t BuOK (mmol)	V (mL) ^b	Yield (%) ^c	2a (mol%)	H ₂ (ppm) ^d	H ₂ (mol%) ^e
0	none	0.75	15.5	<5 (2.3)	-	968	0.1
1	6 mol% FeCl ₂	0.75	15.4	> 99 (99.6)	trace	16.0×10 ⁴	20.1

2	6 mol% FeCl ₃	0.75	15.2	> 99 (99.6)	trace	14.6×10 ⁴	18.1
3	18 mol% FeCl ₂	1.05	15.2	96.4	trace	19.0×10 ⁴	23.6
4	18 mol% FeCl ₃	1.05	13.7	92.7	trace	18.8×10 ⁴	21.0
5	30 mol% FeCl ₂	1.35	14.6	84.3	8.4	22.4×10 ⁴	26.7
6	30 mol% FeCl ₃	1.35	14.4	68.1	23.7	16.1×10 ⁴	18.9

^aGeneral reaction conditions: **1a** (0.5 mmol, 1 equiv), **2a** (0.6 mmol), ^tBuOK (0.75 mmol), 1 mL of THF, dry nitrogen atmosphere, metal: ligand = 1: 2.4.

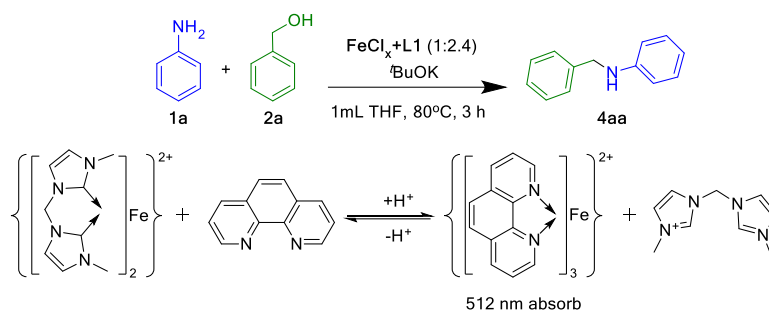
^bGas volume in Schlenk tube (Volume of added liquid to full fill the Schlenk tube).

^cYield was determined by GC analysis with FID and 1,3,5-trimethoxybenzene as standard.

^dHydrogen was determined by GC analysis with TCD.

^eH₂ (mol%) = H₂ (ppm) × V (mL) / (24.5 (mL / mmol) × 0.5 mmol).

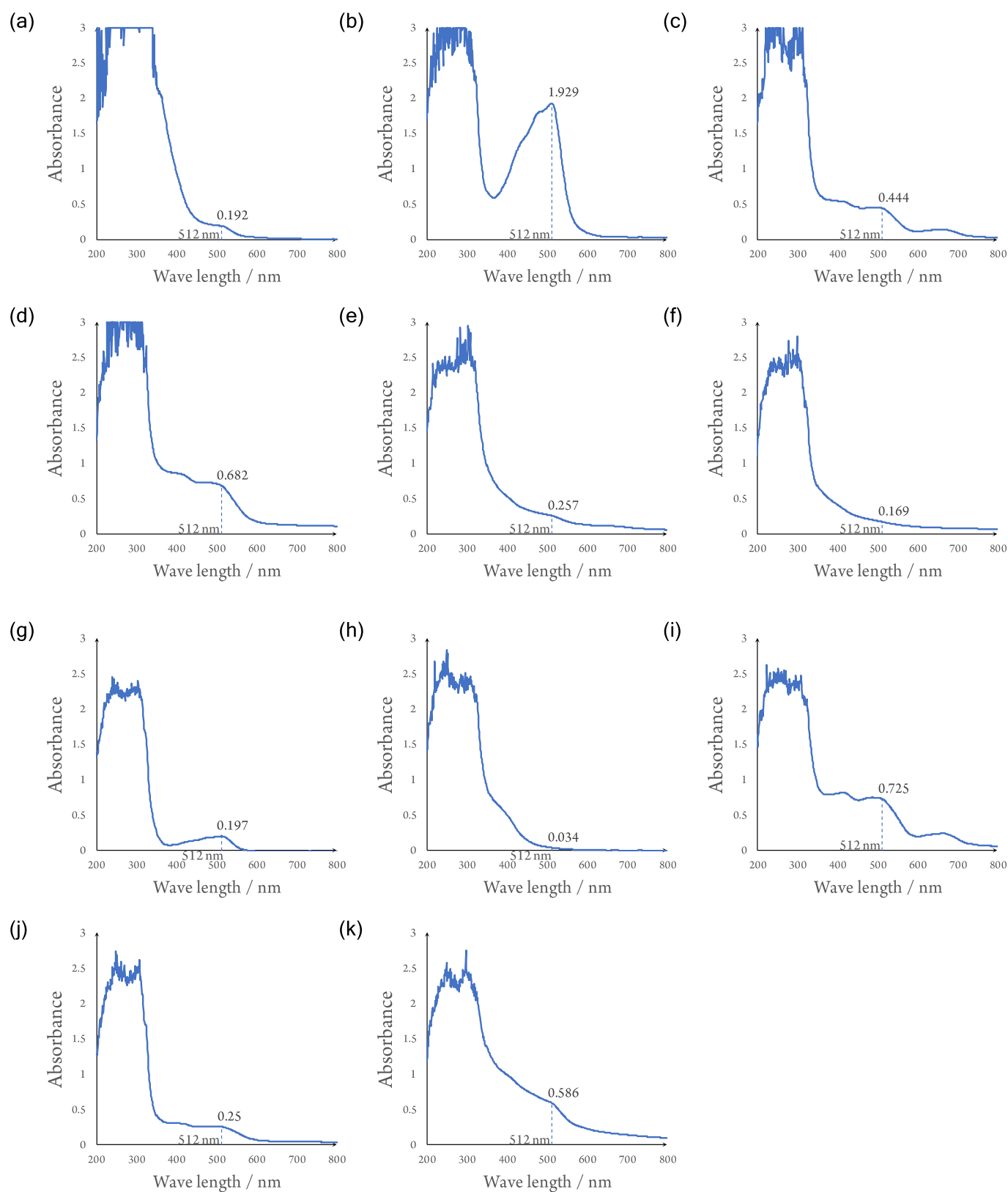
Table S5. UV-Vis Spectrophotometers for Reaction Solutions^a



entry	Aniline	Benzyl alcohol	<i>t</i> BuOK	L1	FeCl _x	Abs (512nm)	Figure S1
1	0	0	0	0	18.0 mol% FeCl ₃	0.192	(a)
2	0	0	0	0	18.0 mol% FeCl ₂	1.929	(b)
3	0.5 mmol	0.6 mmol	1.05 mmol	43.2 mol%	18.0 mol% FeCl ₃	0.444	(c)
4	0	0.6 mmol	1.05 mmol	43.2 mol%	18.0 mol% FeCl ₃	0.682	(d)
5	0.5 mmol	0	1.05 mmol	43.2 mol%	18.0 mol% FeCl ₃	0.257	(e)
6	0.5 mmol	0.6 mmol	0	43.2 mol%	18.0 mol% FeCl ₃	0.169	(f)
7	0.5 mmol	0.6 mmol	1.05 mmol	0	18.0 mol% FeCl ₃	0.197	(g)
8	0.5 mmol	0.6 mmol	1.05 mmol	43.2 mol%	0	0.034	(h)
9	0.5 mmol	0.6 mmol	1.35 mmol	72.0 mol%	30.0 mol% FeCl ₃	0.725	(i)
10	0	0	1.05 mmol	43.2 mol%	18.0 mol% FeCl ₃	0.250	(j)
11	0	0	1.05 mmol	43.2 mol%	18.0 mol% FeCl ₂	0.586	(k)

^a General reaction conditions: **1a** (0.5 mmol, 1 equiv), **2a** (0.6 mmol), *t*BuOK (1.05 mmol - 1.35 mmol), 1 mL of THF, dry nitrogen atmosphere, metal: ligand = 1: 2.4, react for 3 hours. After the reaction mixture was cooled to room temperature, 100 μL reaction solution was taken in a 25 mL volumetric flask, 5 mL water was added to dilute it. Then, 2 mL of 0.1 mol/L HCl, 10 mL of 0.008 mol/L 1,10-Phenanthroline, 2 mL of 1 mol/L sodium acetate were added in order. Finally, water was added to dilute to scale. 2 mL of liquid in the volumetric flask was added to a 10 mm pathlength quartz cell and spectral absorbance was measured with a laboratory benchtop spectrophotometer between 200 and 800 nm.

Figure S1. UV-Vis Spectrophotometers for Reaction Solutions between 200 and 800 nm.



10. X-ray Photoelectron Spectrum

Table S6. Fitting parameters for high resolution XPS Fe 2p spectra of the dried reaction solution.

Band	Position (eV)	Separation (eV)	FWHM (eV)	% Gaussian
Fe ^{II} 2p _{3/2}	708.0	0	1.43	80
Satellite	711.4	3.4	2.95	80
Fe ^{II} 2p _{1/2}	721.6	13.6	2.96	80
Satellite	726.3	18.3	3.54	80
Fe ^{III} 2p _{3/2}	709.9	0	1.92	80
Satellite	714.0	4.1	3.2	80
Fe ^{III} 2p _{1/2}	723.5	13.6	4.85	80
Satellite	730.4	20.5	4.73	80

11. Characterization for Metal Hydride.

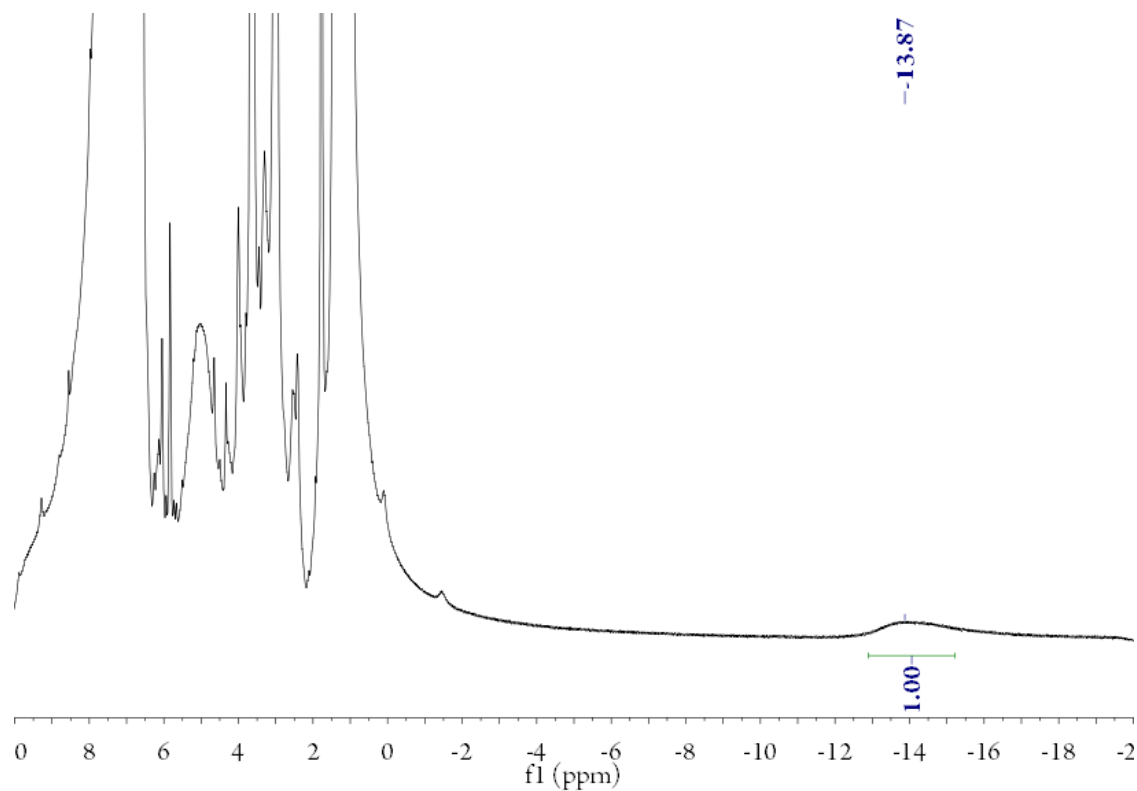
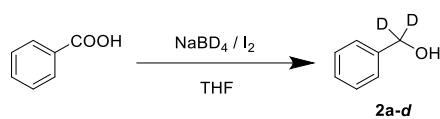


Figure S2. ¹H NMR(C₆D₆) characterization of *in-situ* generated [Fe-H] species.

12. Deuterium Labeling Experiments.

Scheme S4. Synthesis of **1a-d**¹



A 1000 mL round-bottom flask was fitted with a magnetic stir bar, a reflux condenser, and an additional funnel. The flask was charged with NaBD₄ (2.00 g, 48.0 mmol) and THF (80 mL, predried over sodium). Benzoic acid (3.90 g, 32 mmol) was added in one portion. The flask was cooled to 0 °C in an ice bath. A solution of I₂ (8.12 g, 32.0 mmol) in 100 mL of THF was added dropwise over 60 min. After gas evolution had ceased, the flask was heated to reflux for 18 h and then cooled to room temperature, and methanol was added cautiously until the mixture turned clear. After stirring 30 min, the solvent was removed by rotary evaporation leaving a white paste which was dissolved by addition of 20% aqueous KOH (70 mL). The solution was stirred for 4 h and extracted with CH₂Cl₂ (60 mL × 2). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and concentrated under vacuum. The residue **2a-d** (2.52 g) was obtained in 71%.

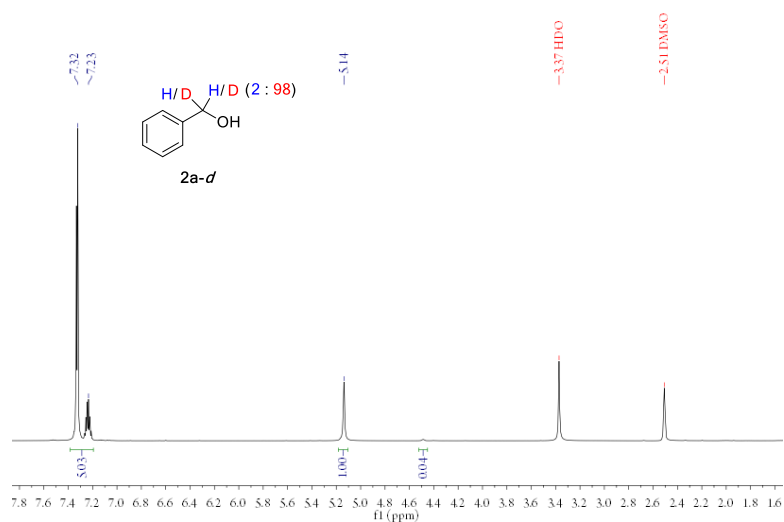


Figure S3. ¹H NMR (DMSO-*d*₆) spectra of the synthetic **2a-d**.

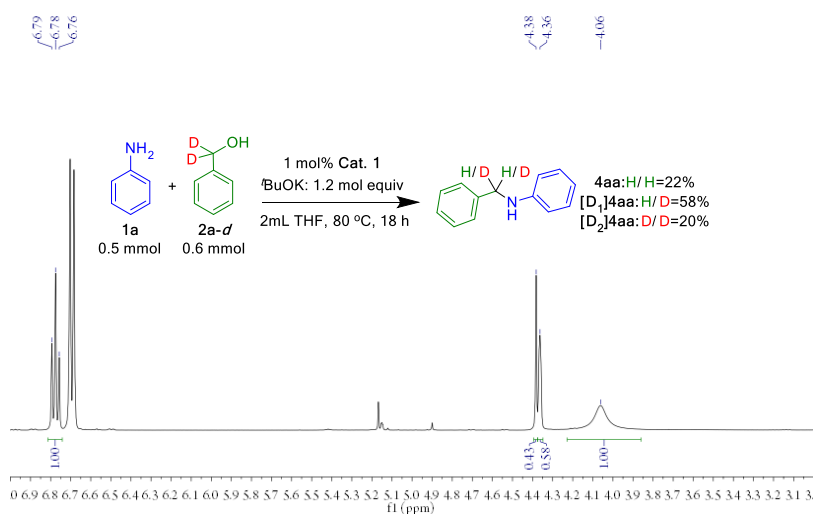


Figure S4. ^1H NMR (CDCl_3) spectra of the products of the reaction of **2a-d** with **1a** in the range of 3-7 ppm.

13. Monitoring the Kinetics of the Reaction.

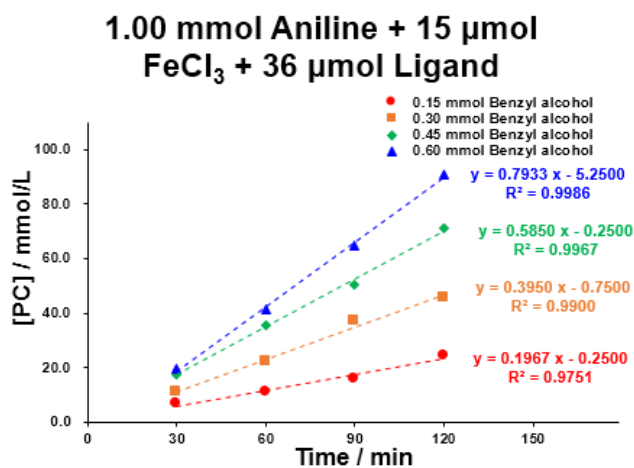


Figure S5. Control experiments for change the amount of benzyl alcohol.

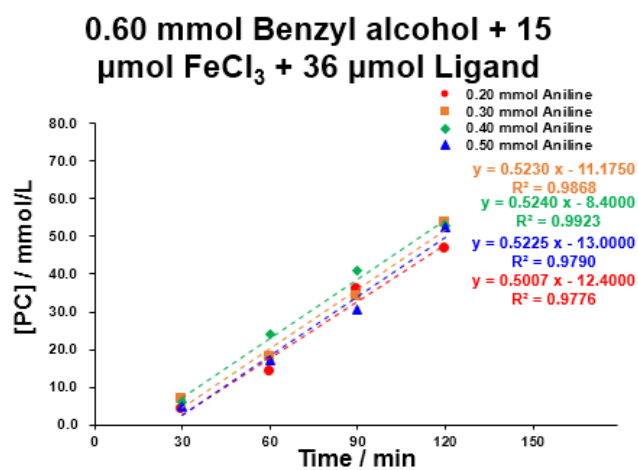


Figure S6. Control Experiments for Change the Amount of aniline.

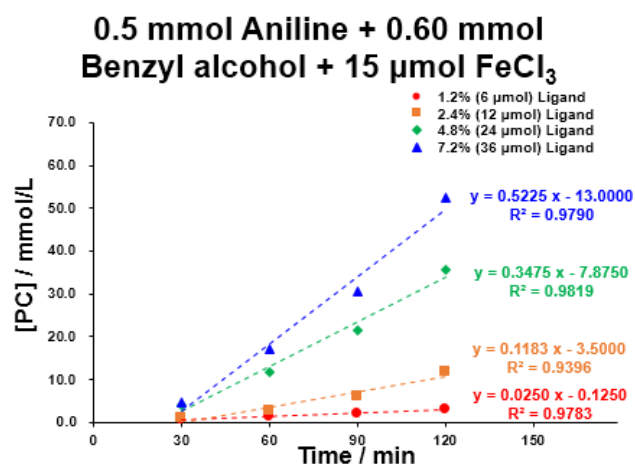


Figure S7. Control experiments for change the amount of FeCl_3 .

0.5 mmol Aniline + 0.60 mmol
Benzyl alcohol + 36 μmol Ligand

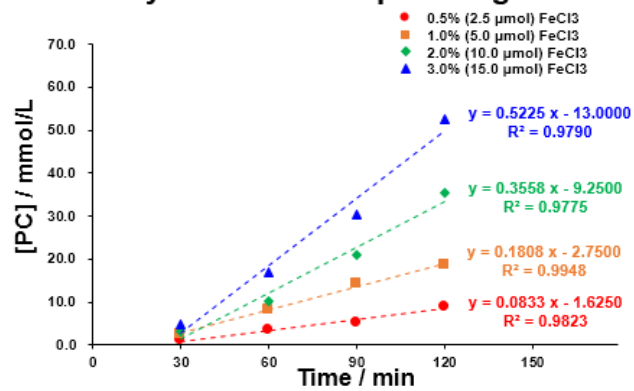
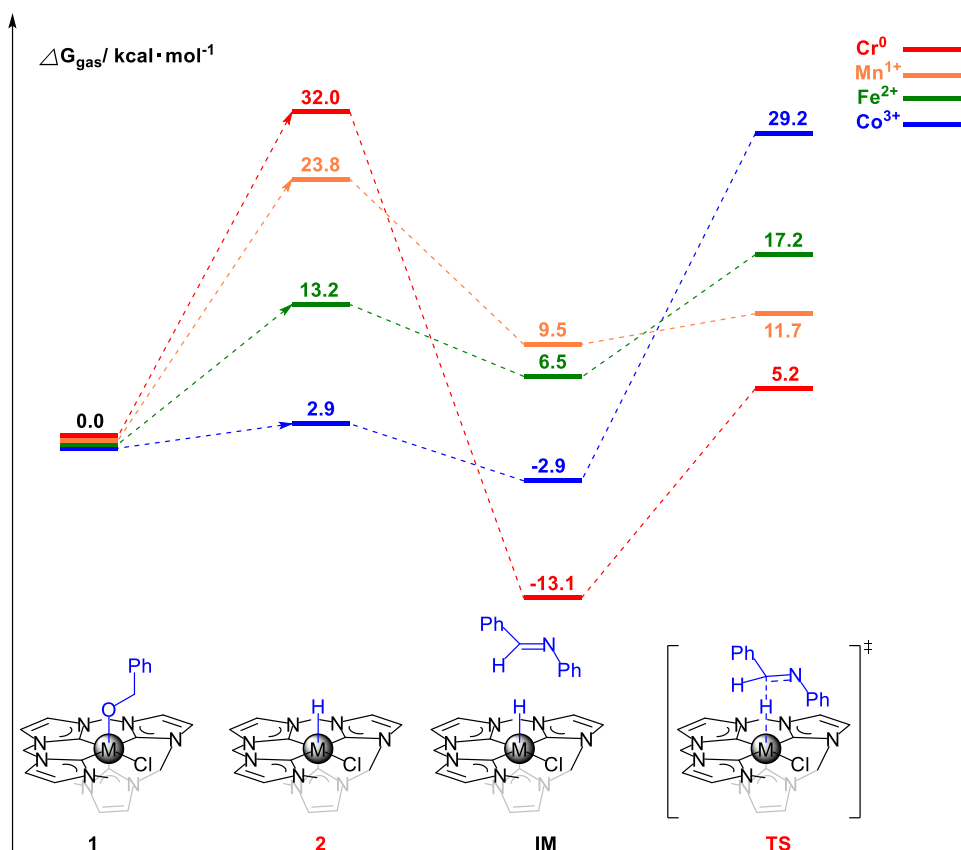


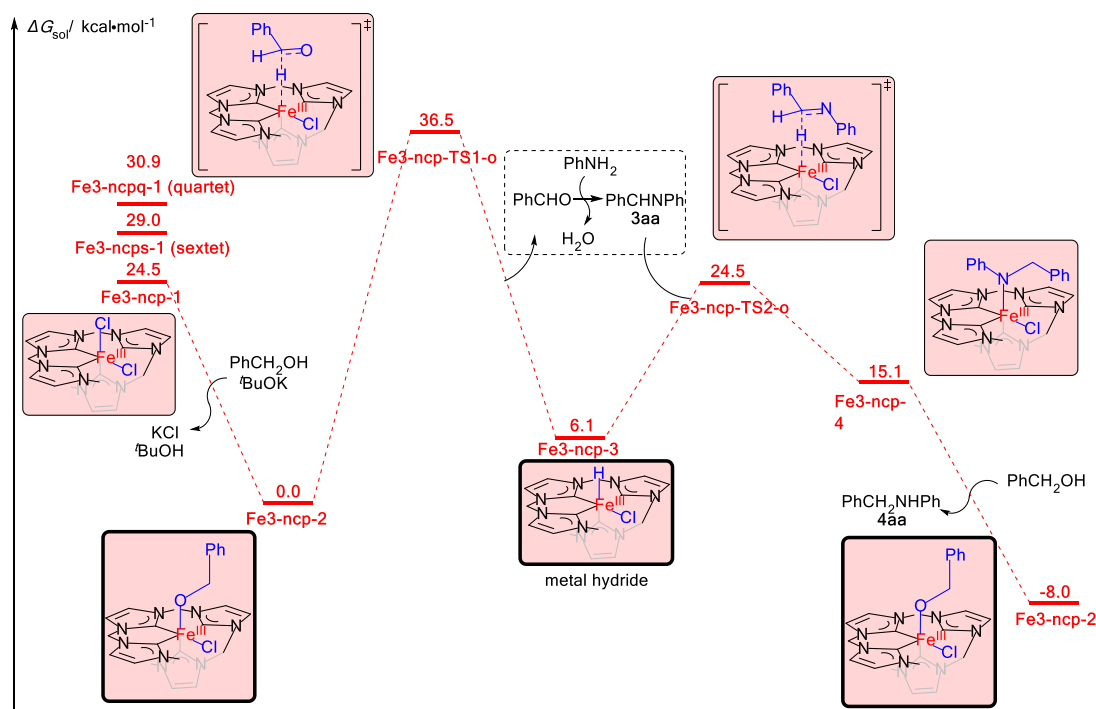
Figure S8. Control experiments for change the amount of L1.

14. DFT Calculations.

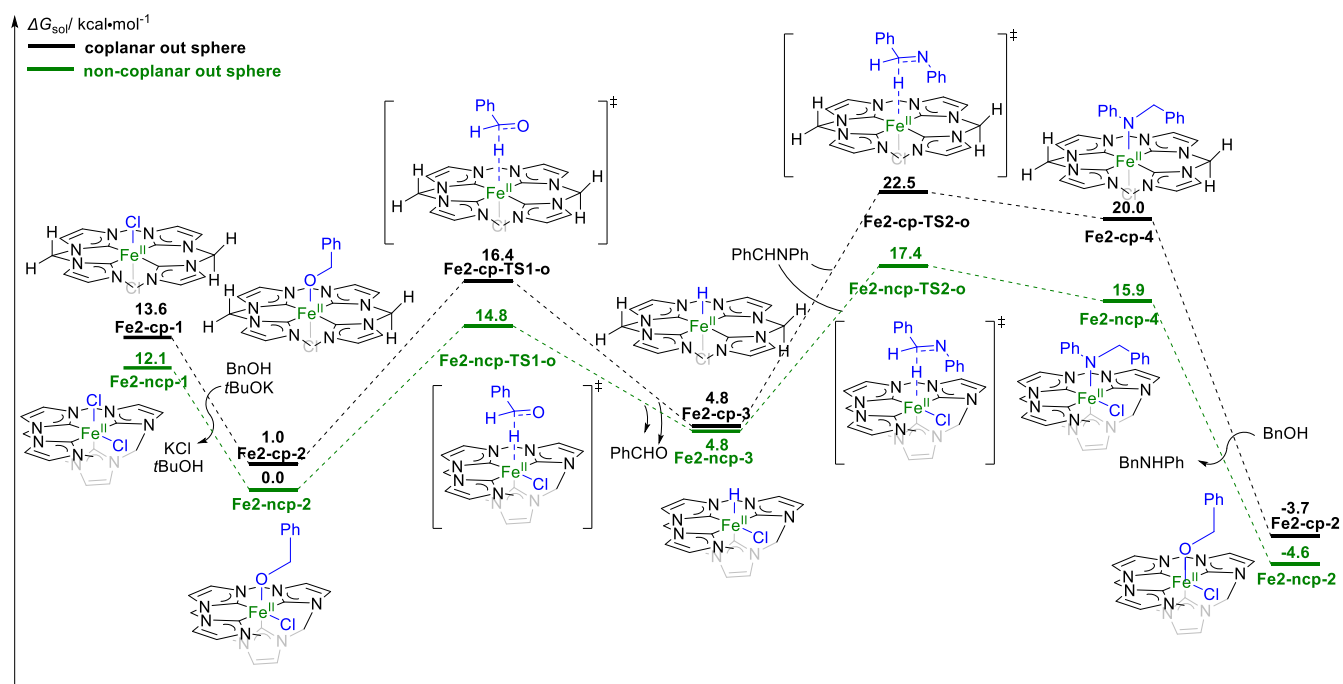
Scheme S5. Comparison of Different Metals for the Metal Hydride and Transition States.



Scheme S6. Proposed Mechanism of Tetracarbone Iron(III) Complex for Catalytic Cycle

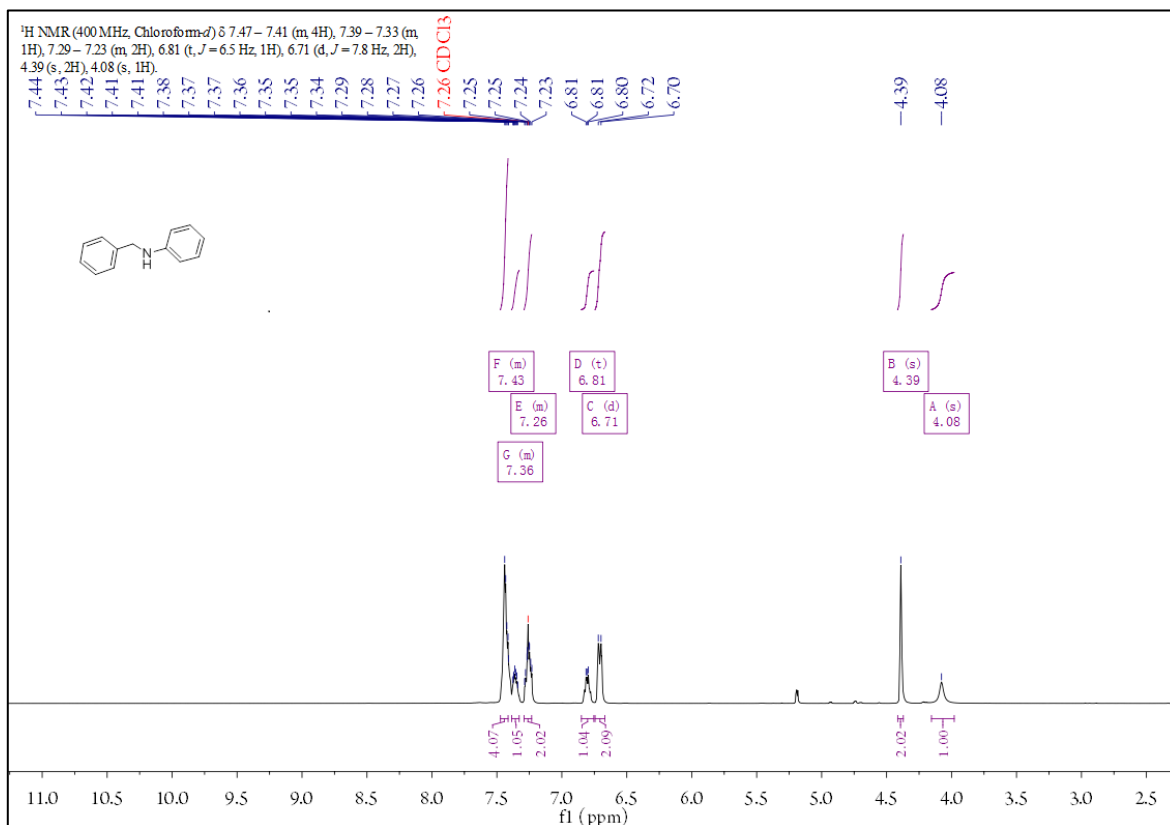


Scheme S7. Proposed Mechanism of Non-coplanar and Coplanar Tetracarbene Iron(II) Complex for Catalytic Cycle

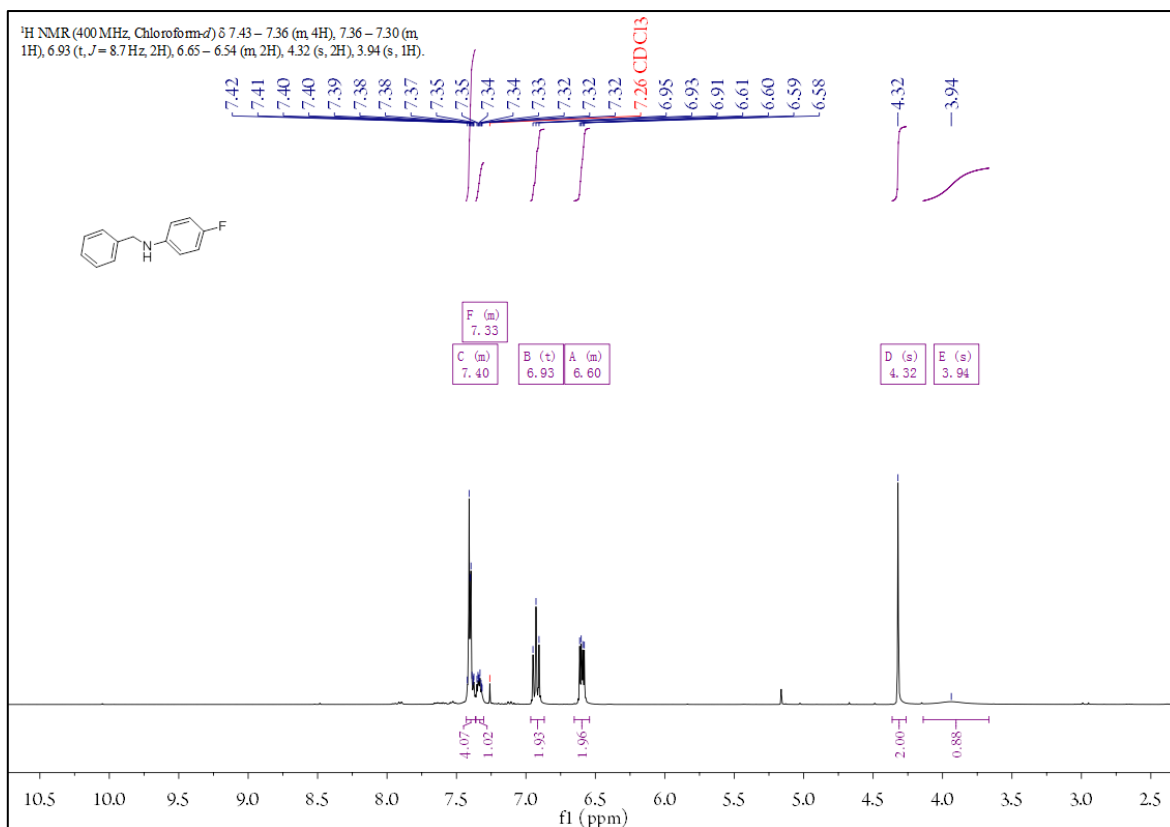


15. NMR spectra of products 4.

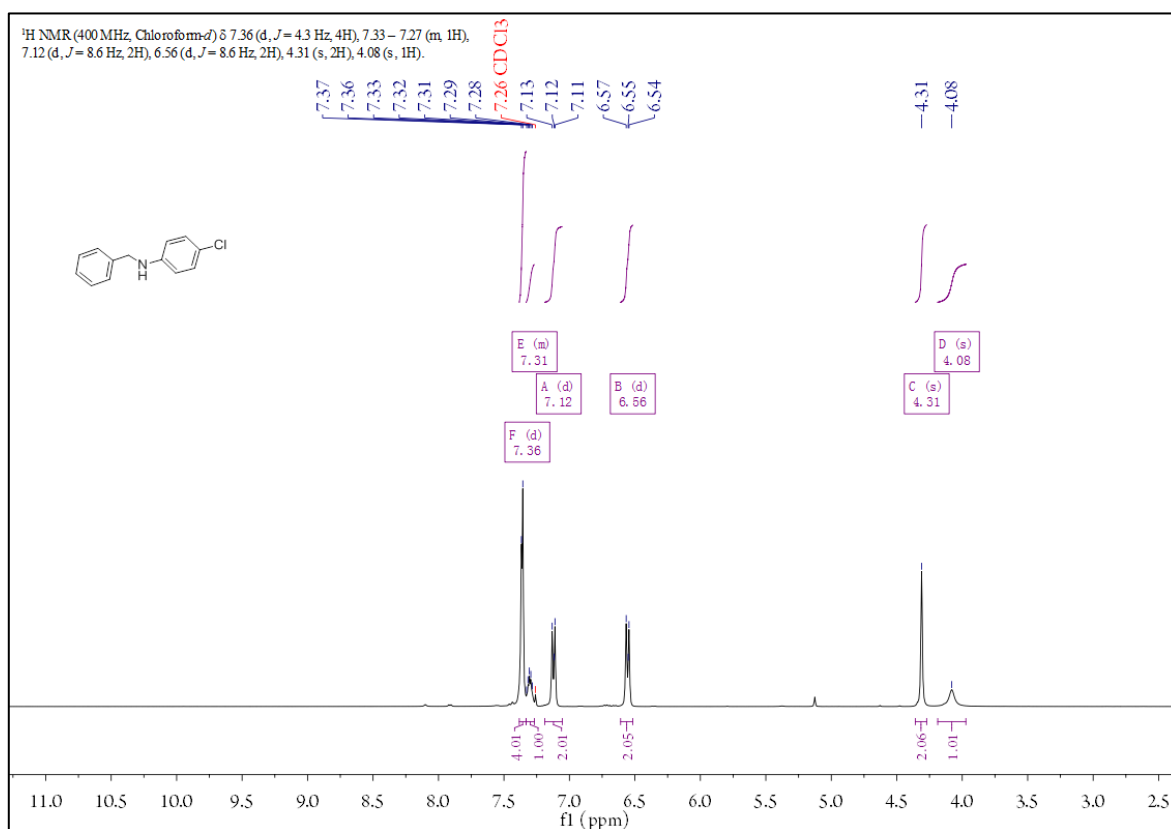
Scheme S8. ¹H-NMR spectrum of 4aa in CDCl₃



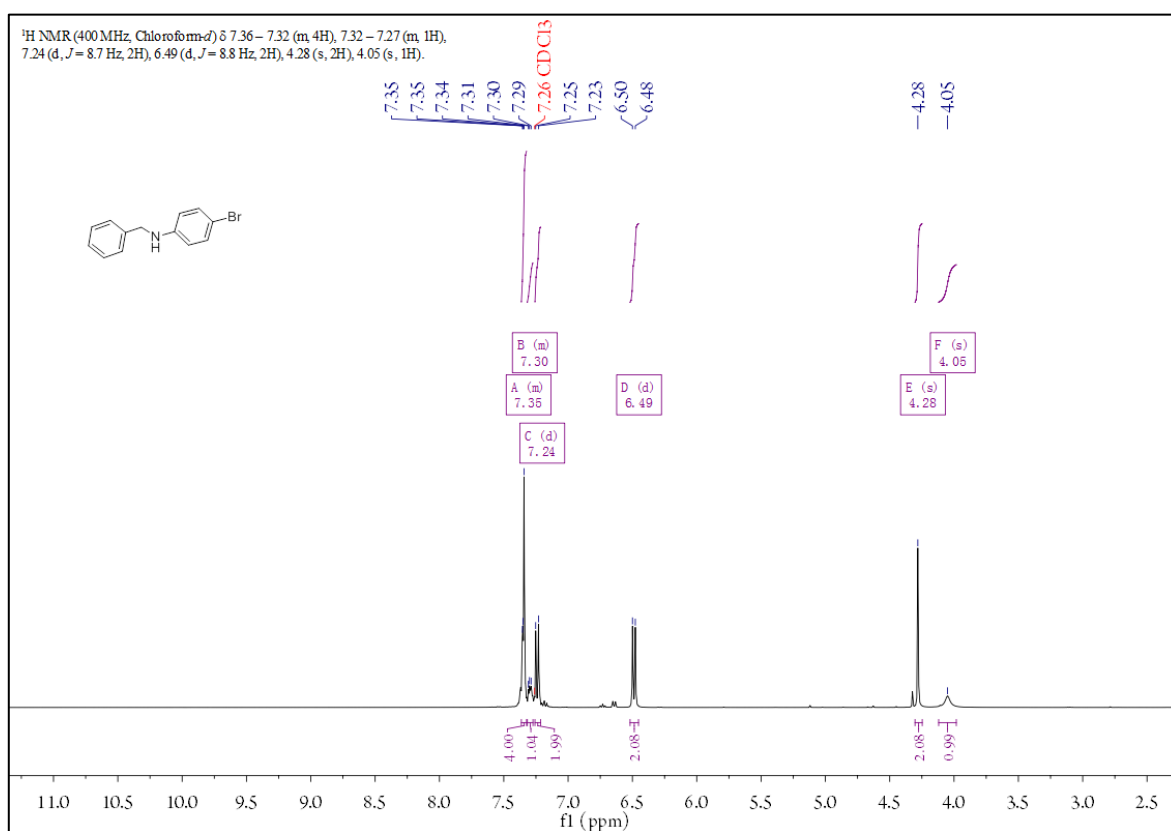
Scheme S9. ¹H-NMR spectrum of 4ba in CDCl₃



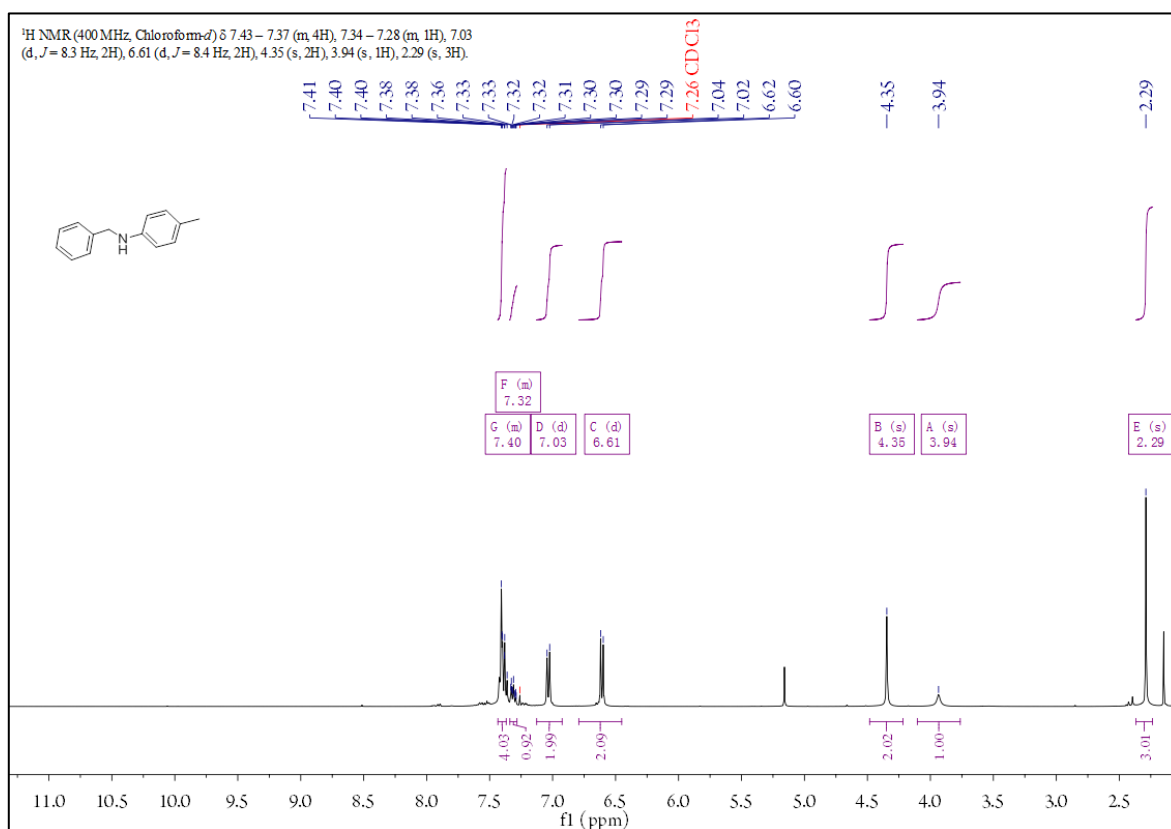
Scheme S10. $^1\text{H-NMR}$ spectrum of 4ca in CDCl_3



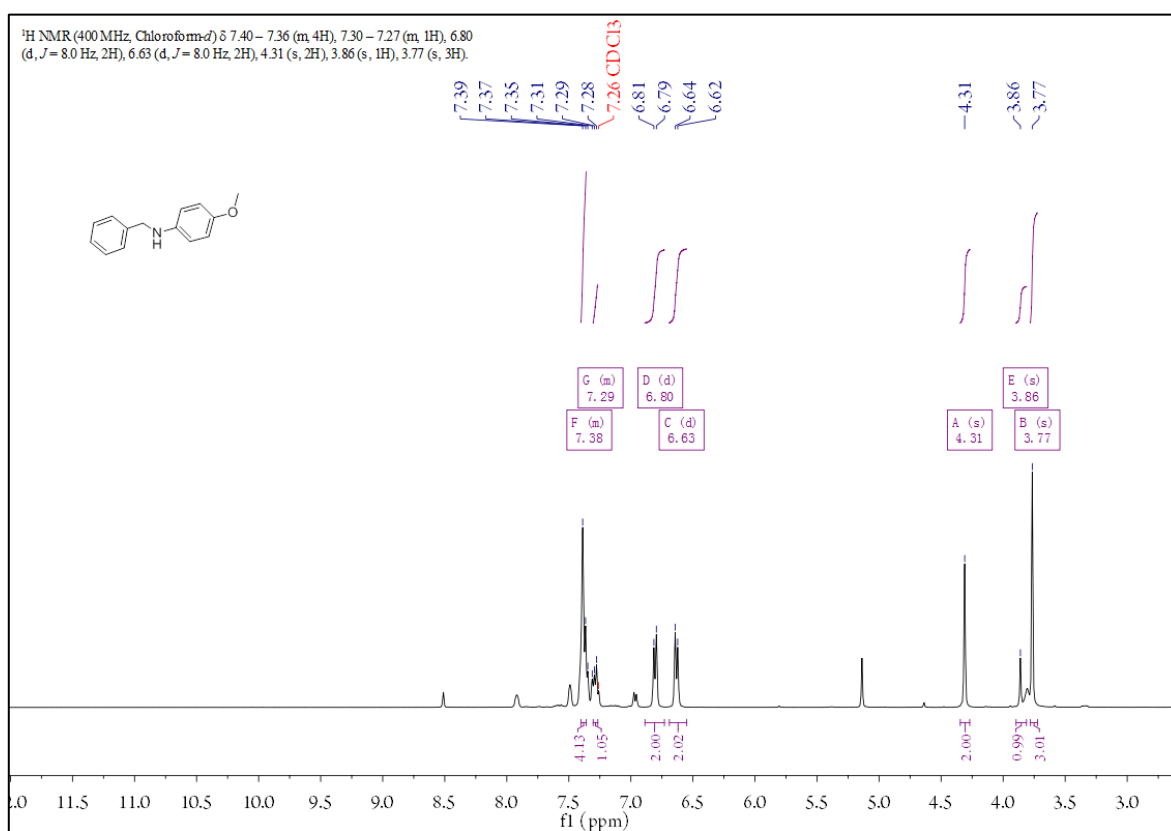
Scheme S11. $^1\text{H-NMR}$ spectrum of 4da in CDCl_3



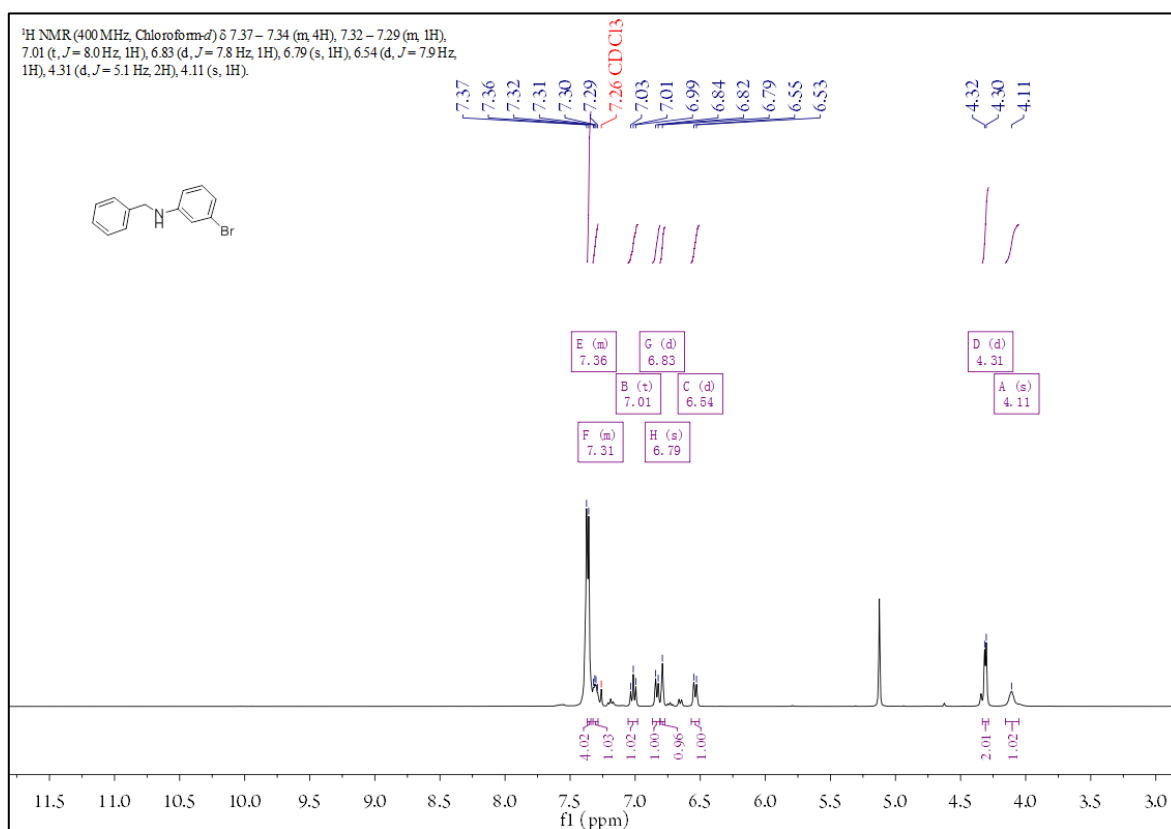
Scheme S12. ¹H-NMR spectrum of 4ea in CDCl₃



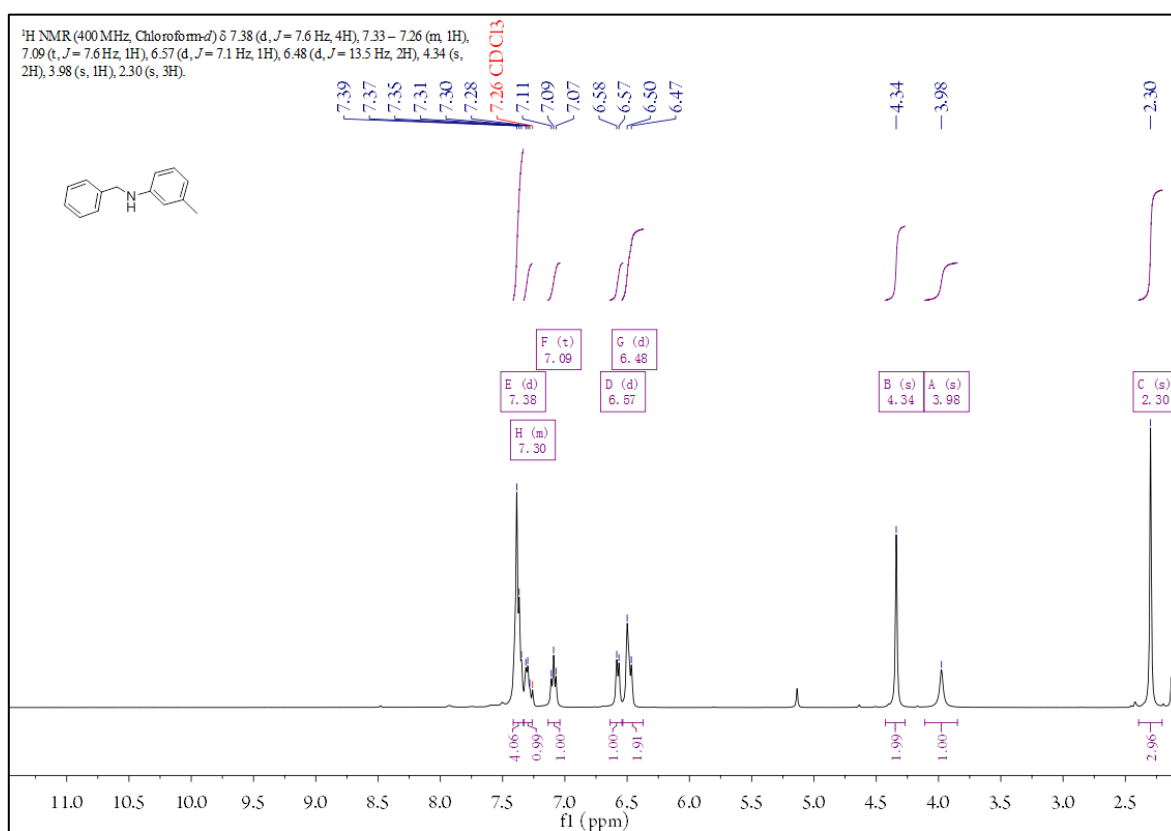
Scheme S13. ¹H-NMR spectrum of 4fa in CDCl₃



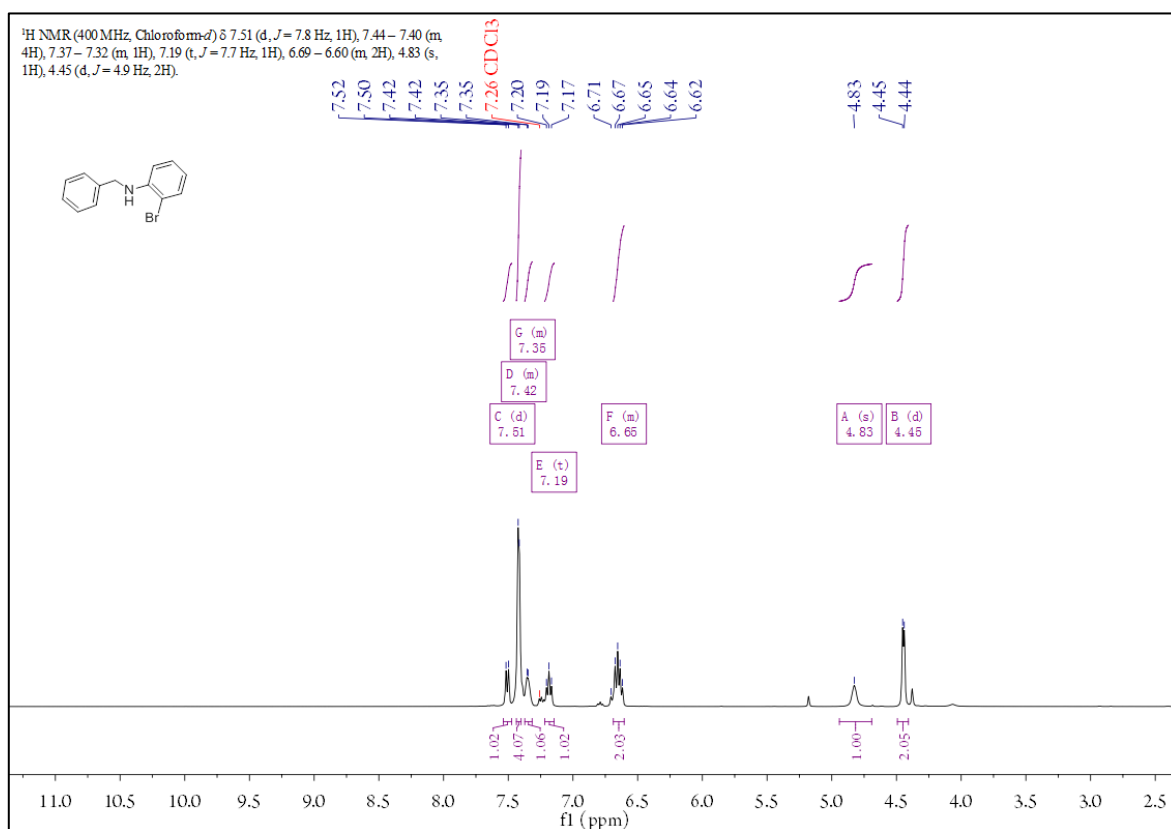
Scheme S14. $^1\text{H-NMR}$ spectrum of 4ga in CDCl_3



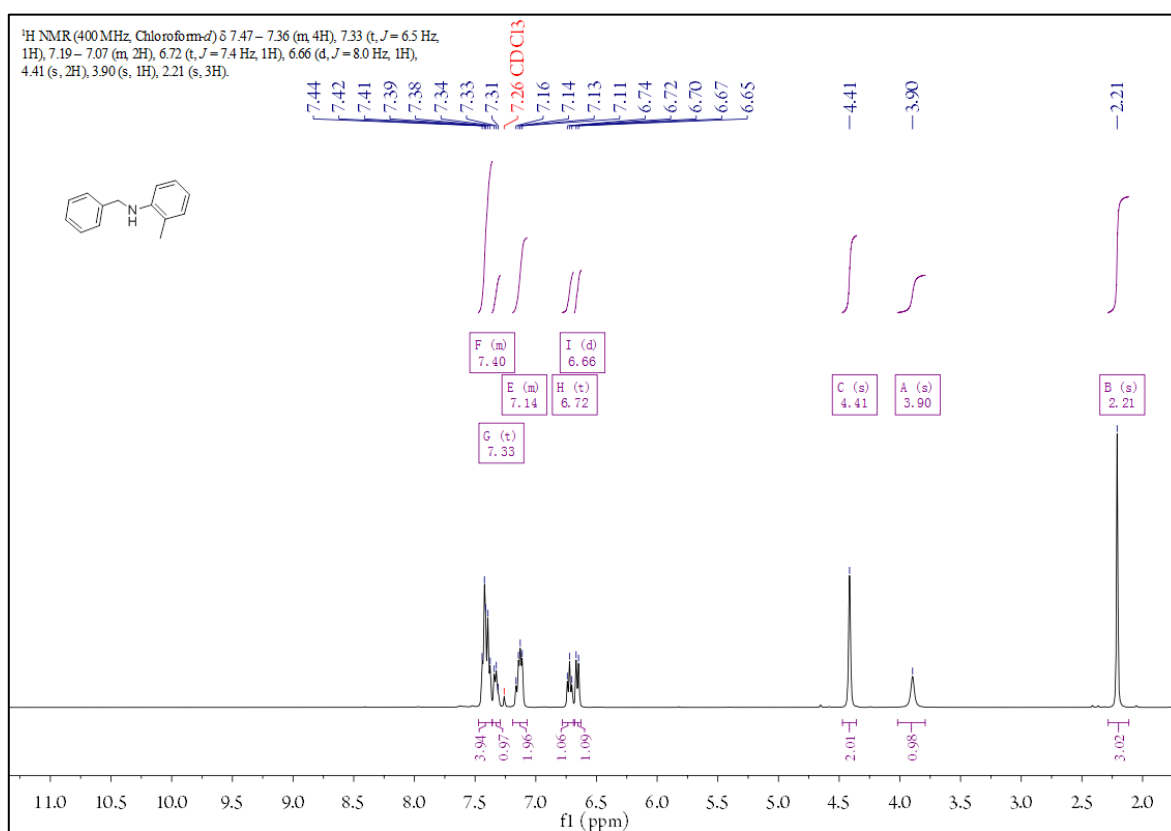
Scheme S15. $^1\text{H-NMR}$ spectrum of 4ha in CDCl_3



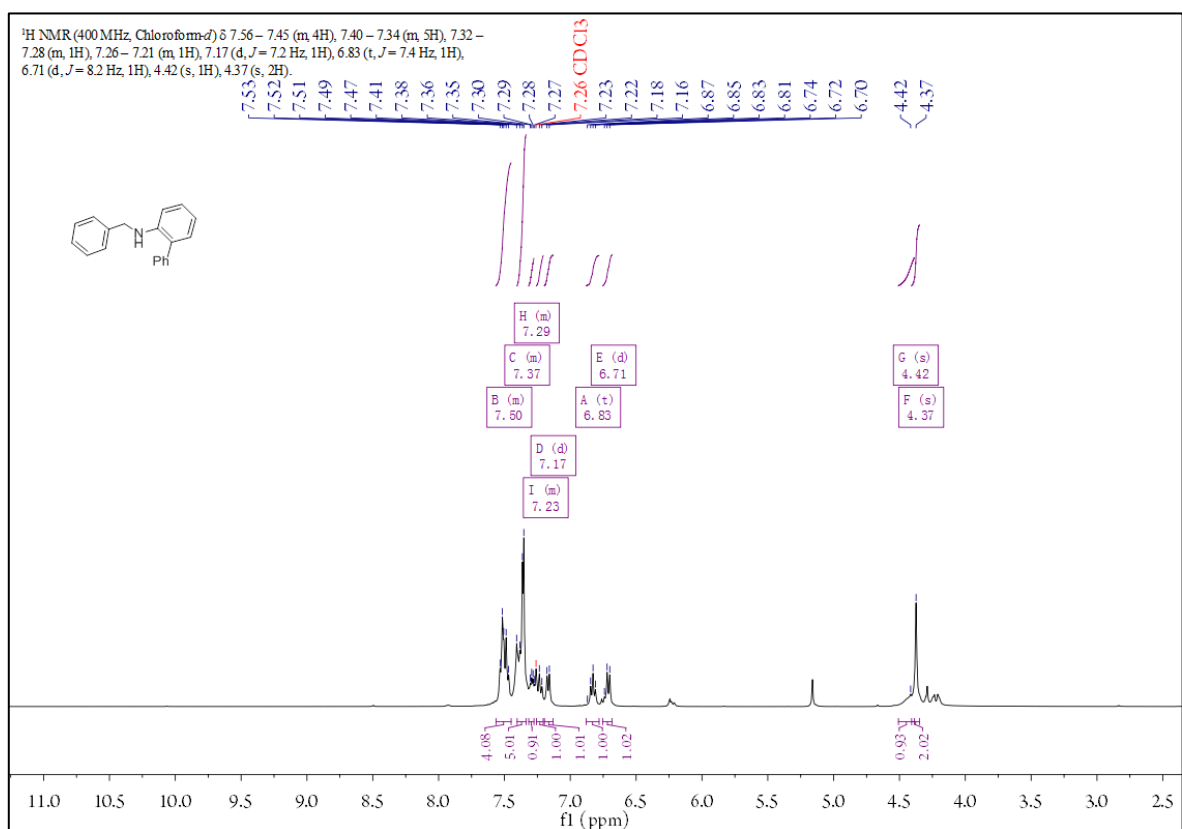
Scheme S16. $^1\text{H-NMR}$ spectrum of 4ia in CDCl_3



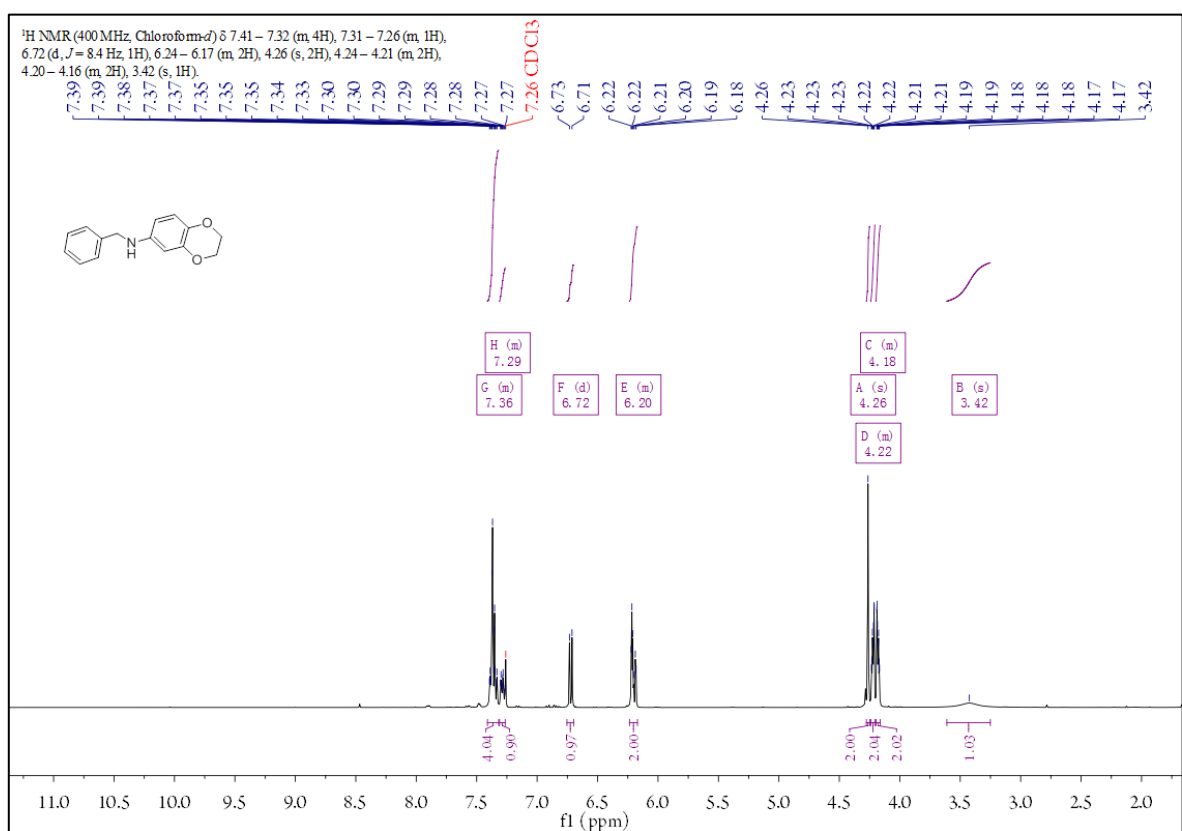
Scheme S17. $^1\text{H-NMR}$ spectrum of 4ja in CDCl_3



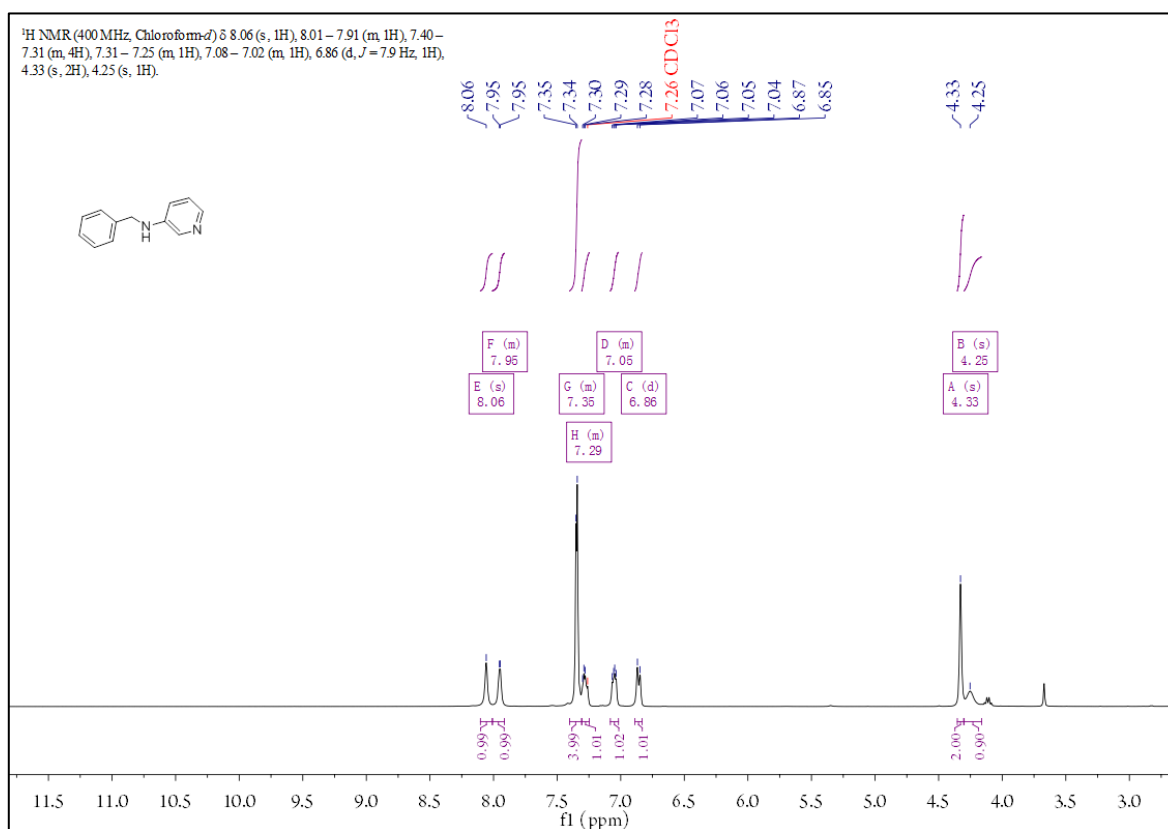
Scheme S18. ¹H-NMR spectrum of 4ka in CDCl₃



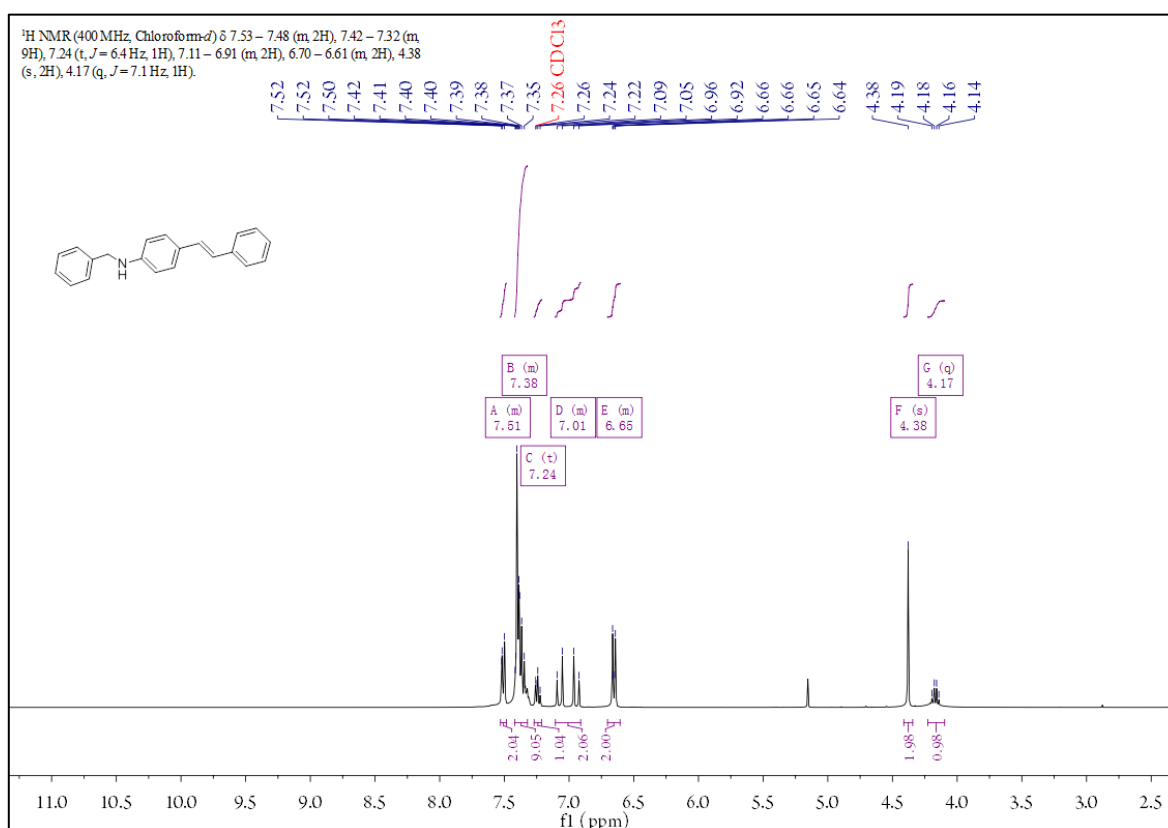
Scheme S19. ¹H-NMR spectrum of 4na in CDCl₃



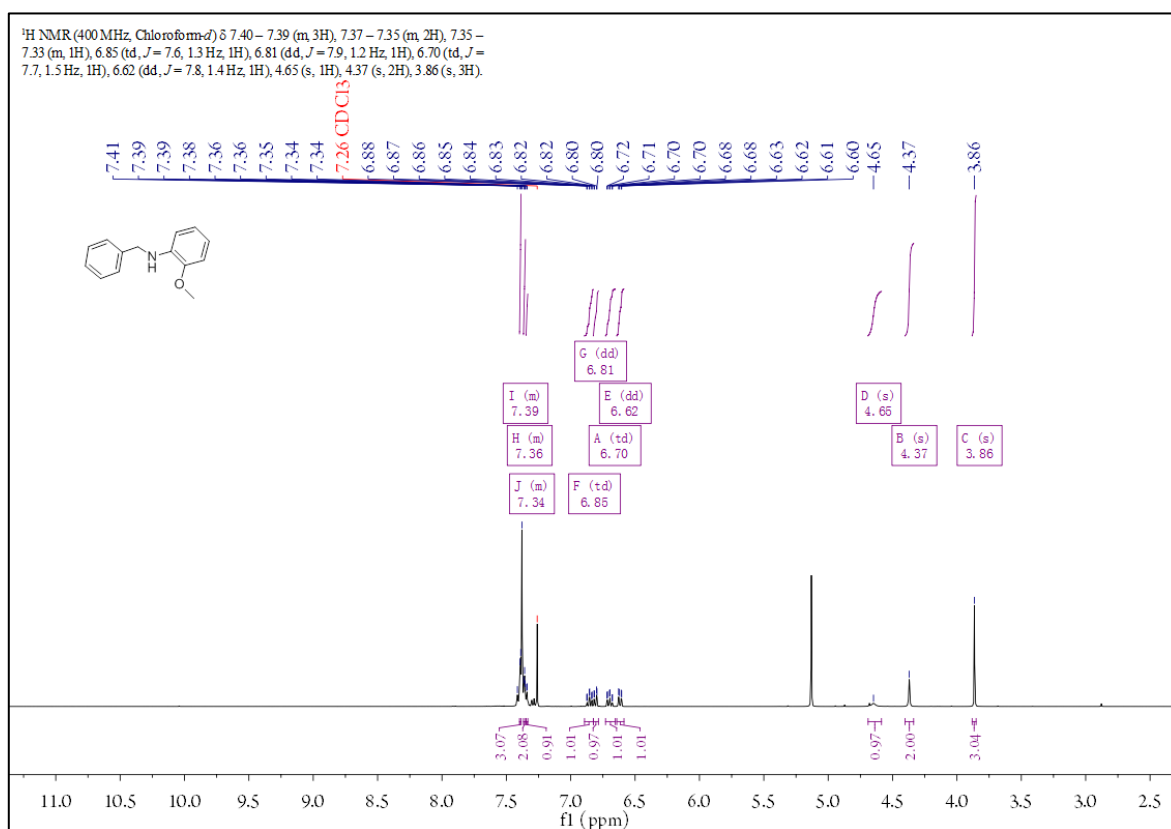
Scheme S20. ¹H-NMR spectrum of 4oa in CDCl₃



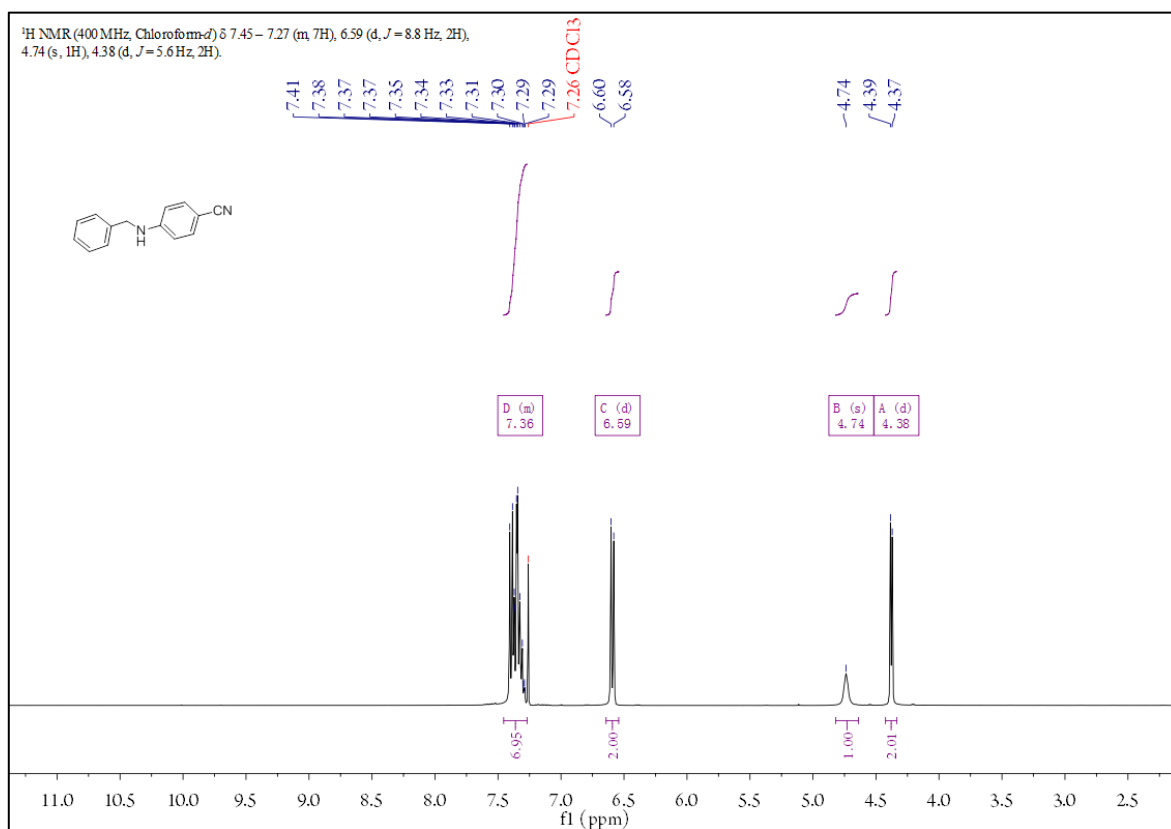
Scheme S21. ¹H-NMR spectrum of 4ra in CDCl₃



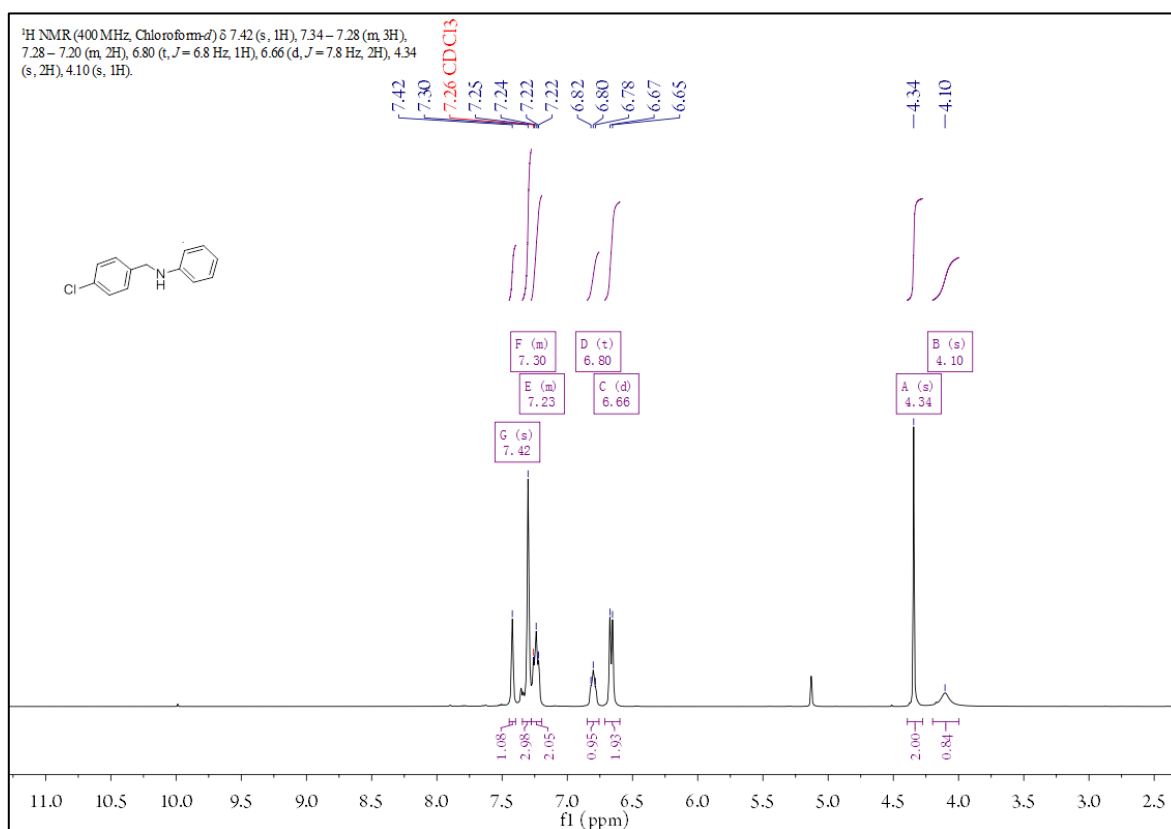
Scheme S22. ¹H-NMR spectrum of 4ta in CDCl₃



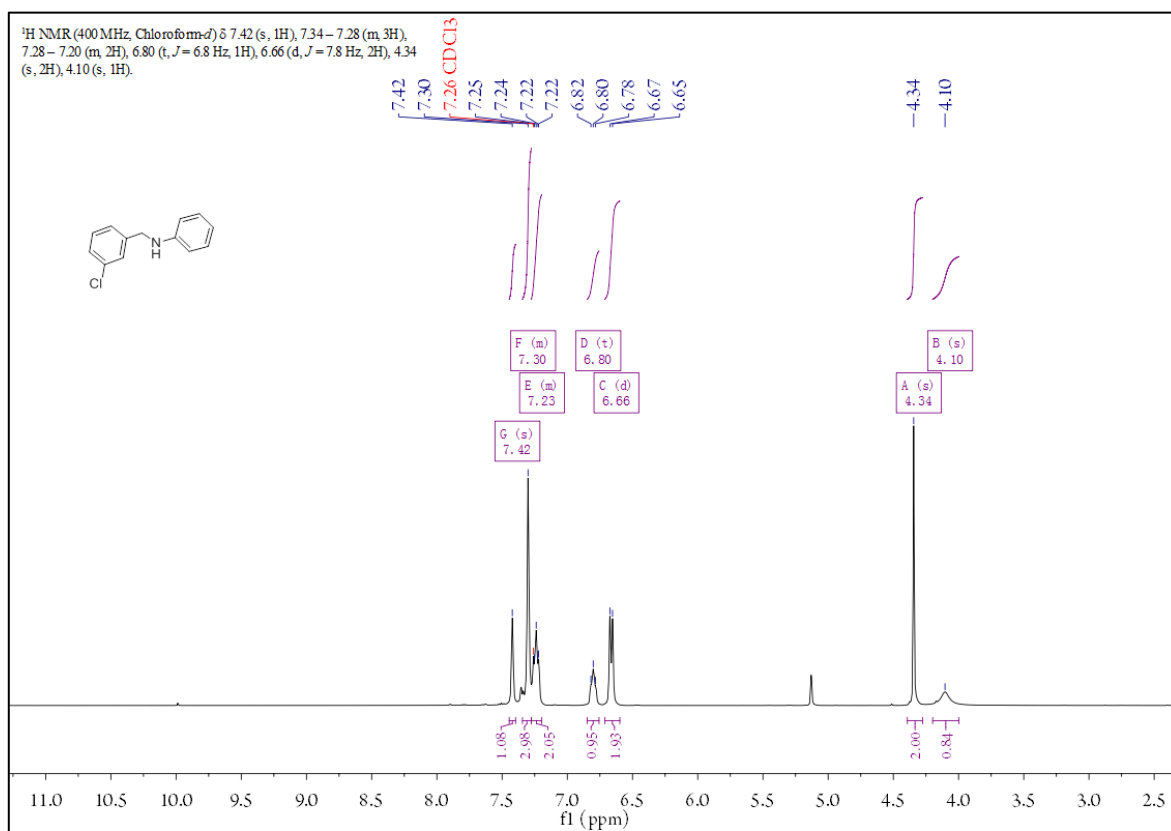
Scheme S23. ¹H-NMR spectrum of 4ua in CDCl₃



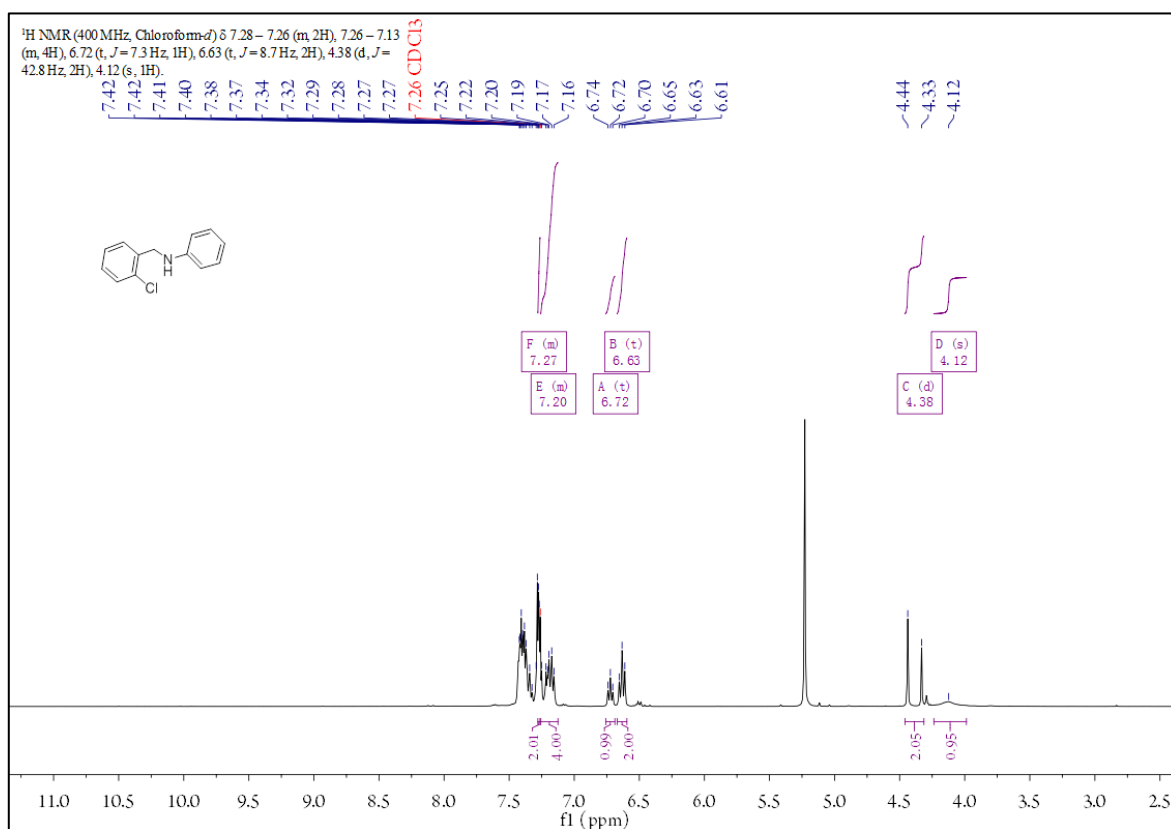
Scheme S24. $^1\text{H-NMR}$ spectrum of 4ab in CDCl_3



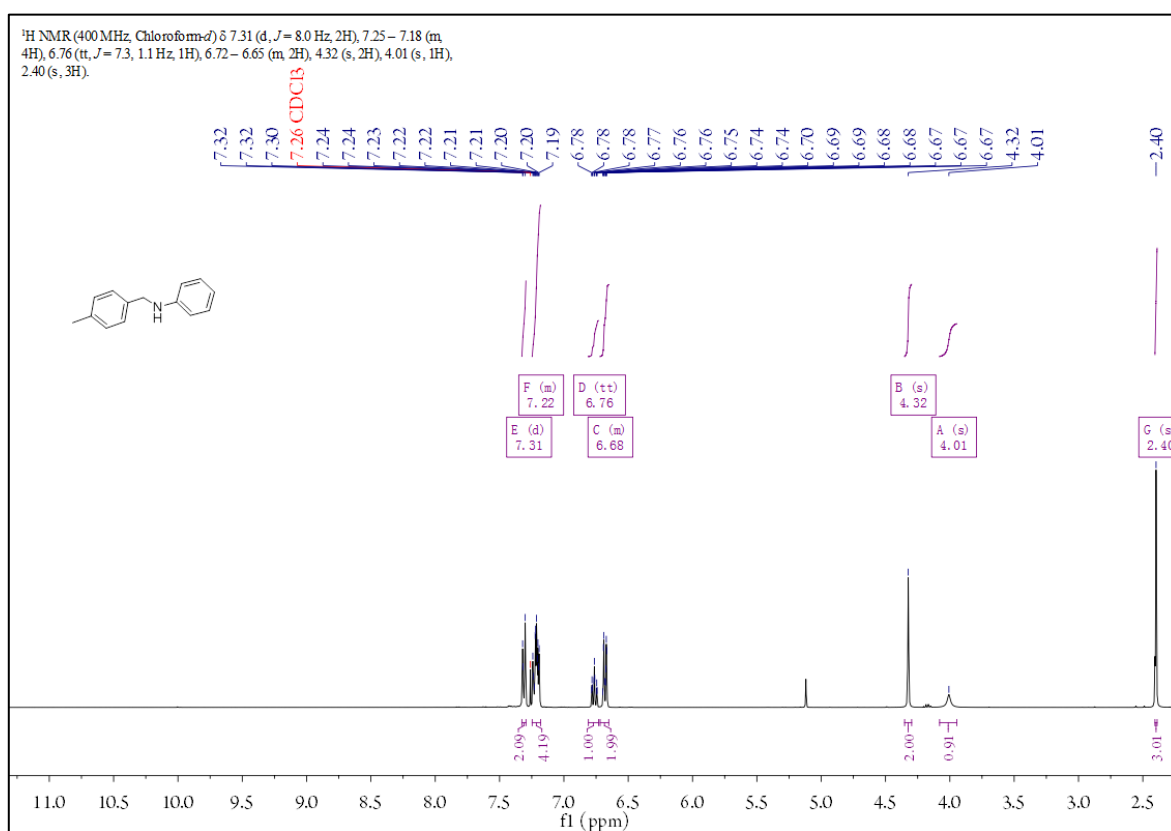
Scheme S25. $^1\text{H-NMR}$ spectrum of 4ac in CDCl_3



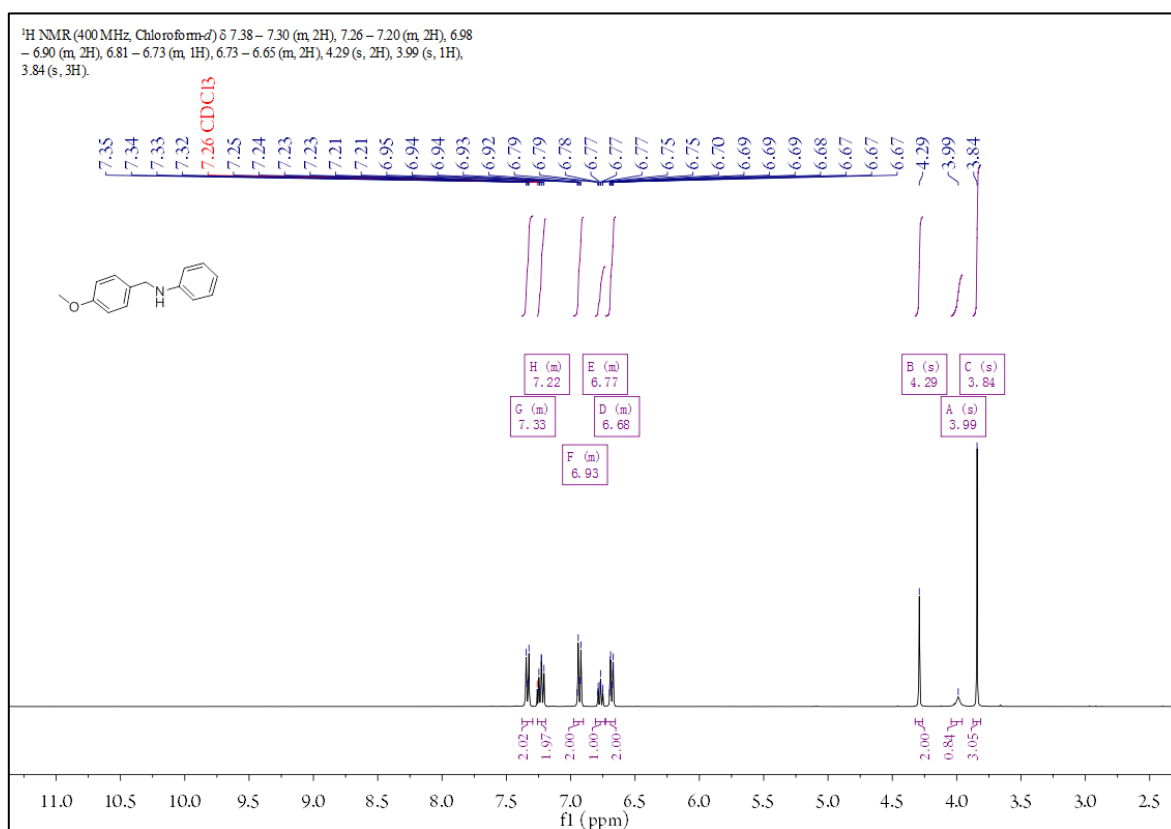
Scheme S26. $^1\text{H-NMR}$ spectrum of 4ad in CDCl_3



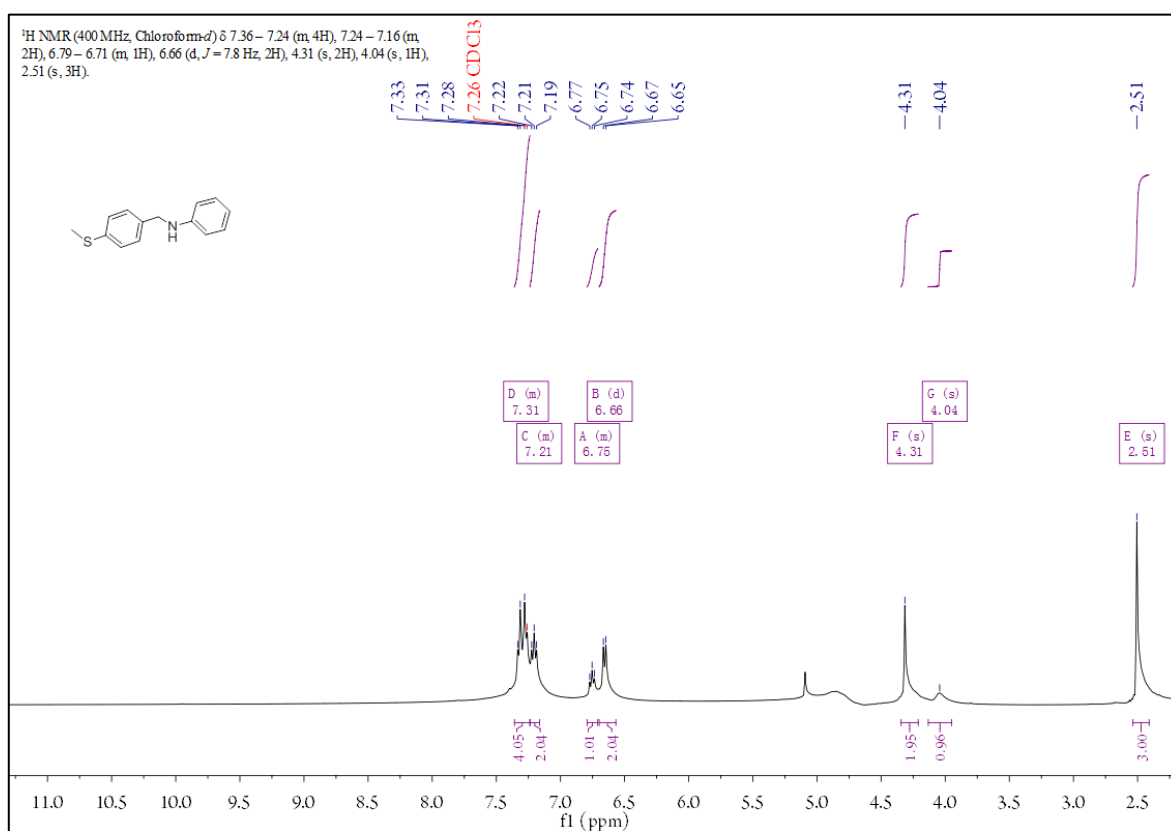
Scheme S27. $^1\text{H-NMR}$ spectrum of 4ae in CDCl_3



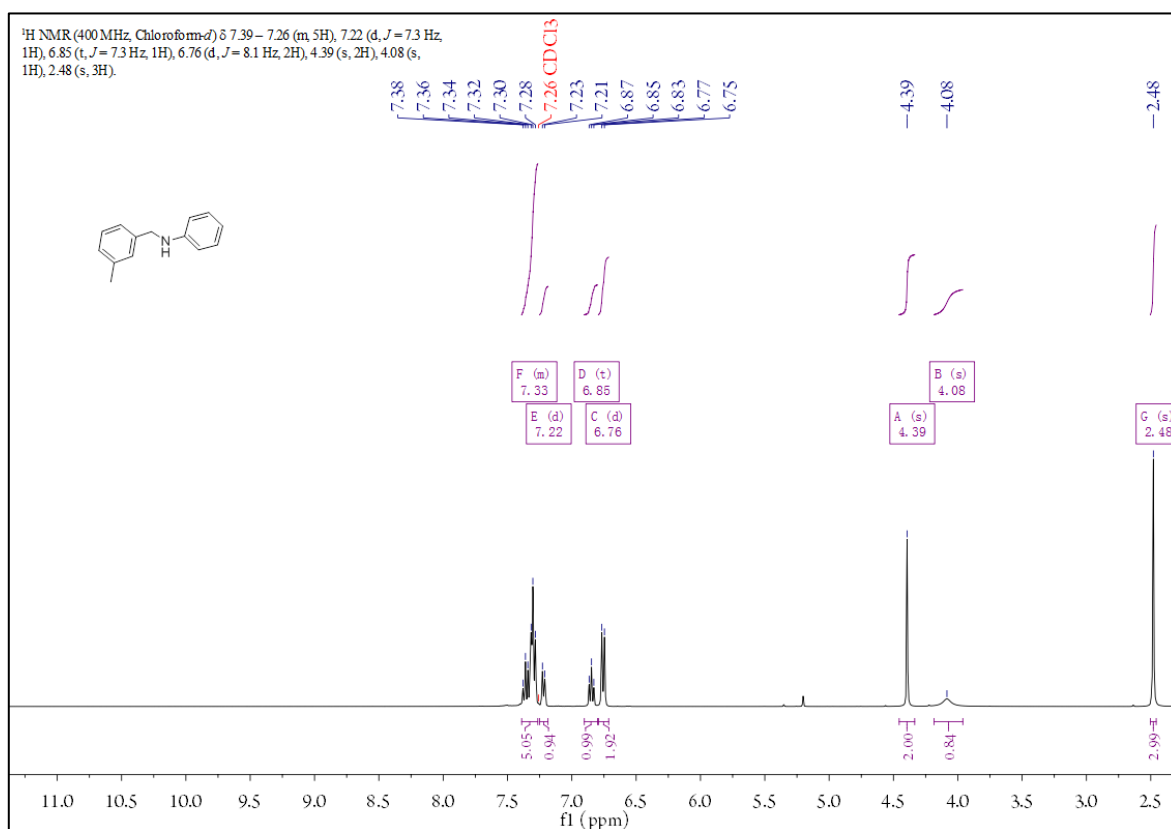
Scheme S28. ¹H-NMR spectrum of 4af in CDCl₃



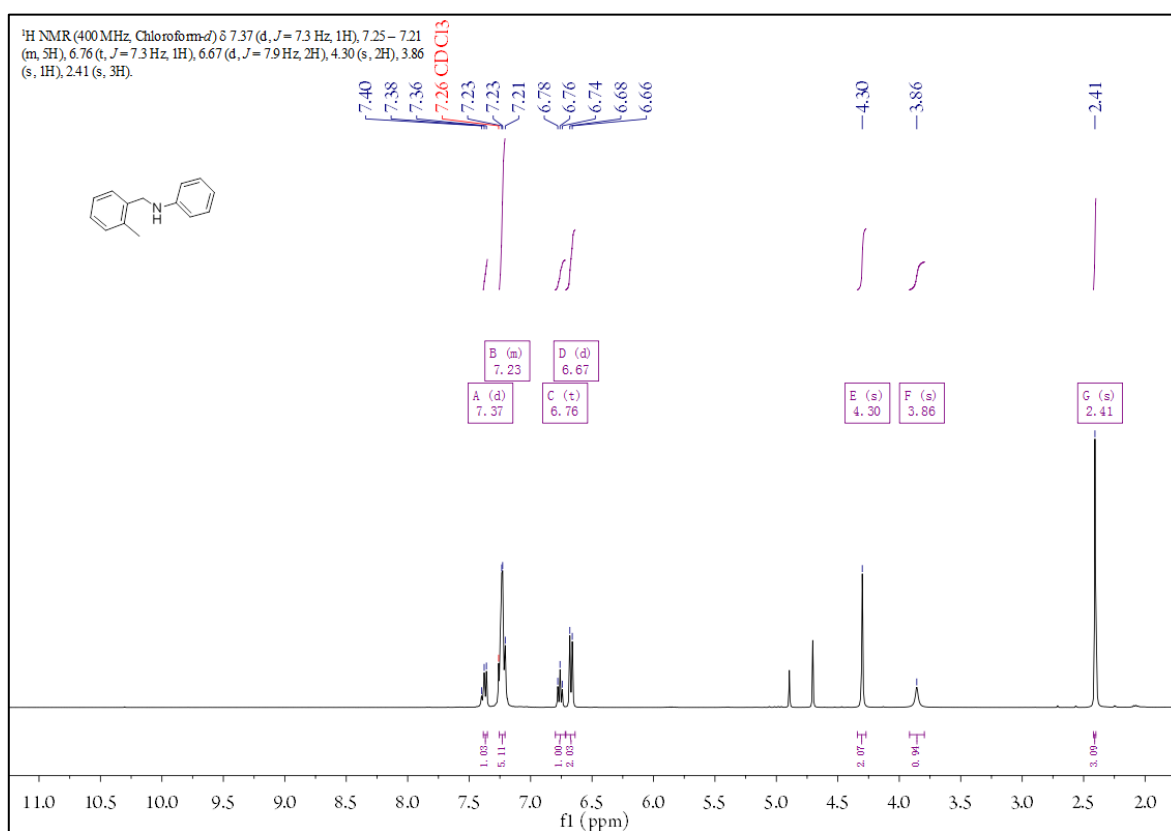
Scheme S29. ¹H-NMR spectrum of 4ag in CDCl₃



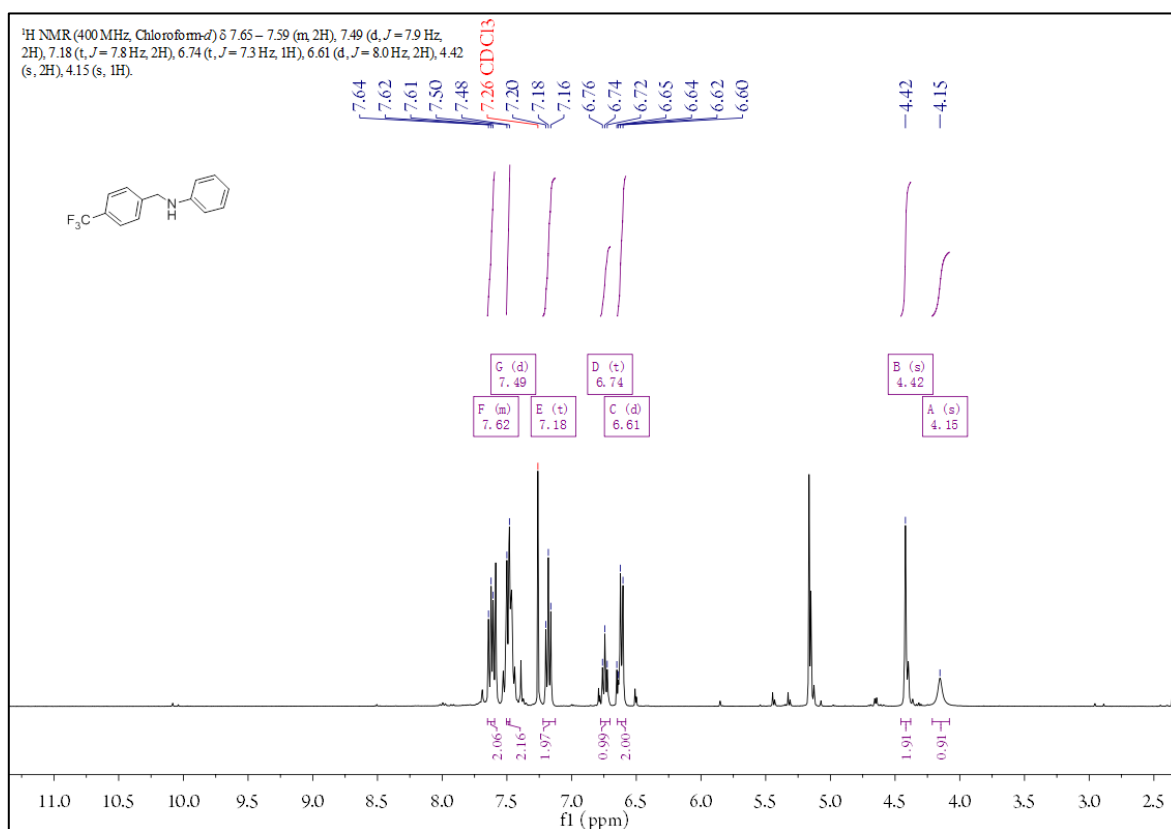
Scheme S30. ¹H-NMR spectrum of 4ah in CDCl₃



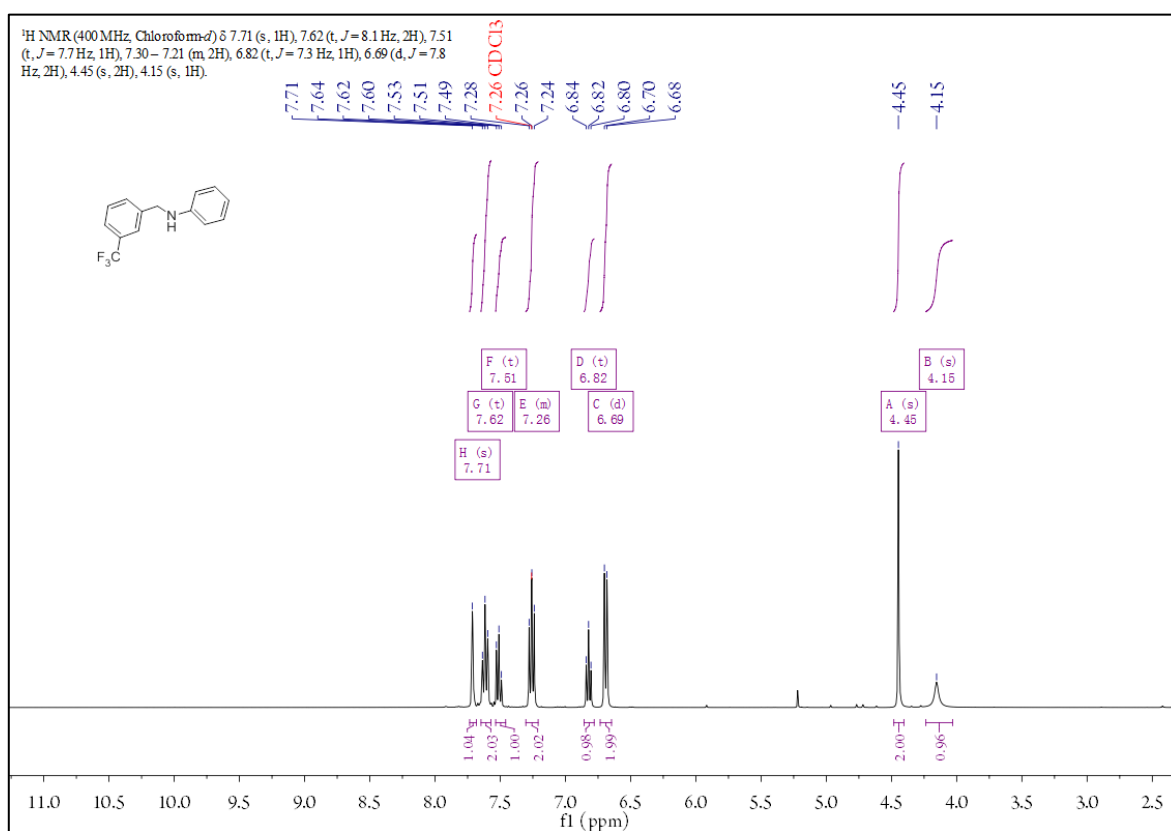
Scheme S31. ¹H-NMR spectrum of 4ai in CDCl₃



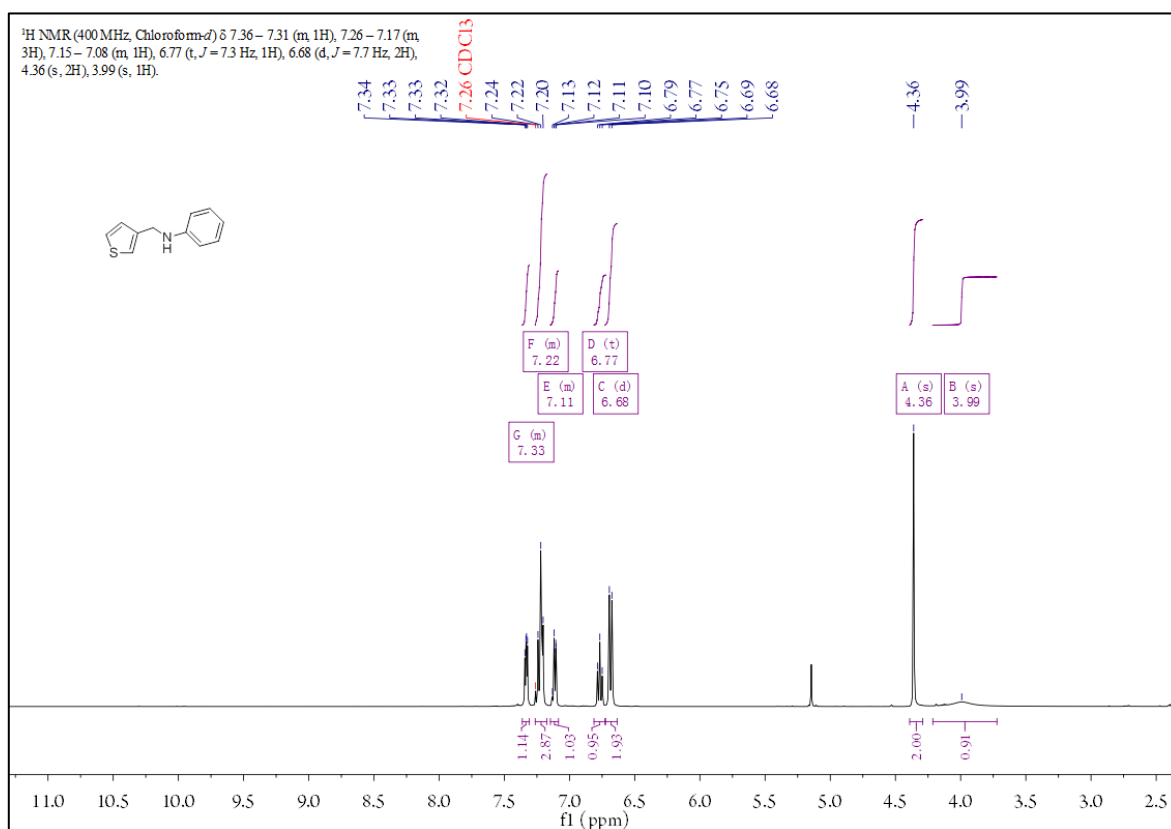
Scheme S32. ¹H-NMR spectrum of 4aj in CDCl₃



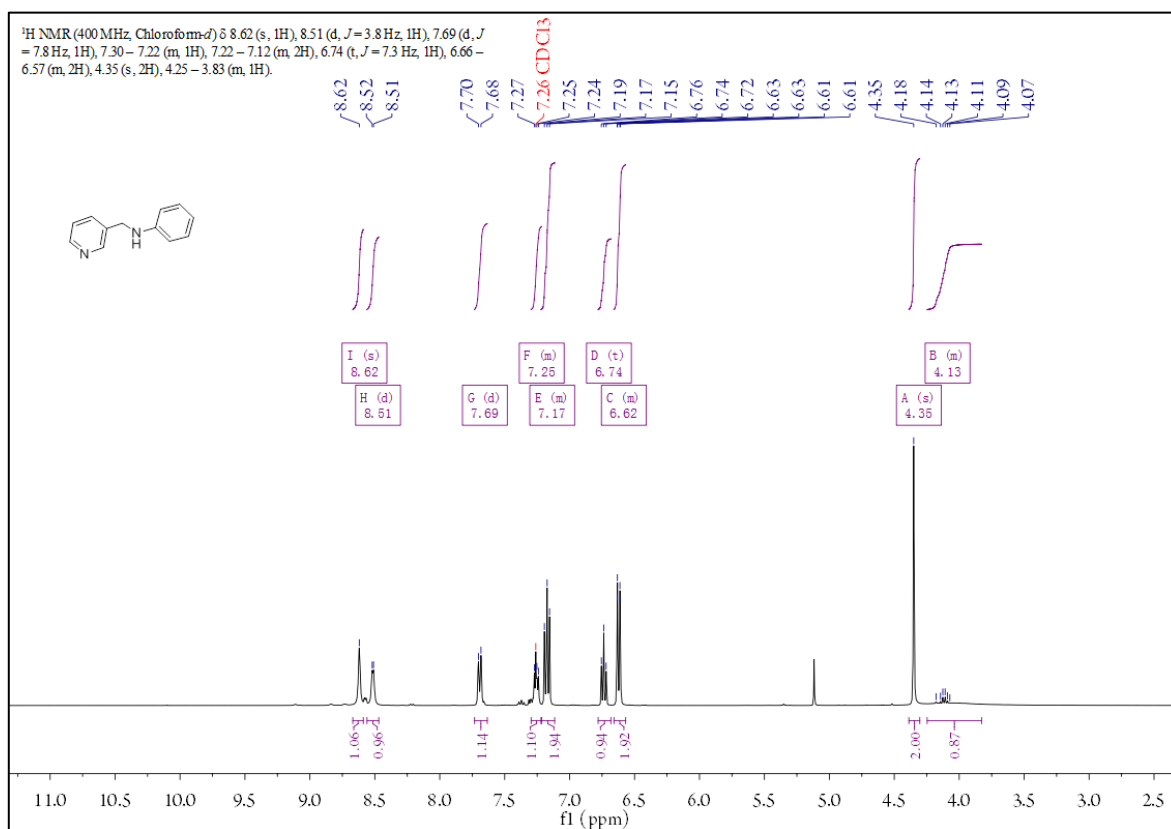
Scheme S33. ¹H-NMR spectrum of 4ak in CDCl₃



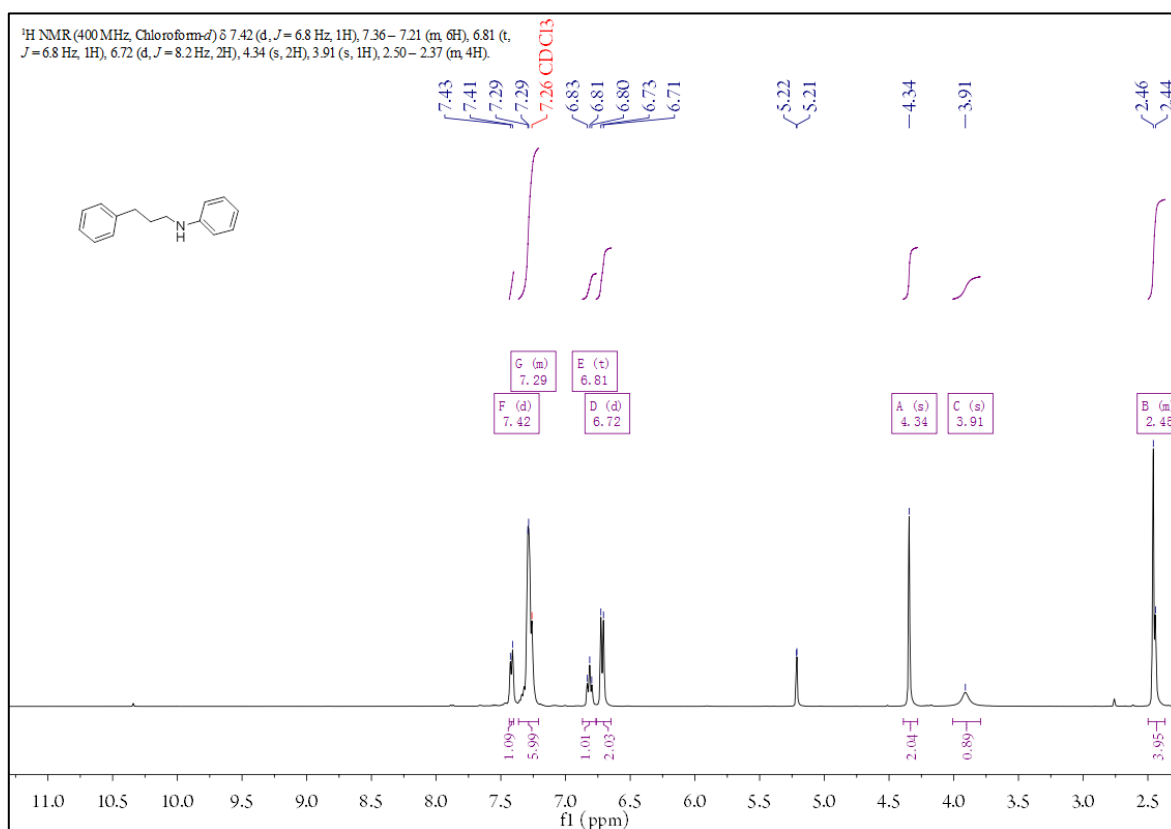
Scheme S34. $^1\text{H-NMR}$ spectrum of 4al in CDCl_3



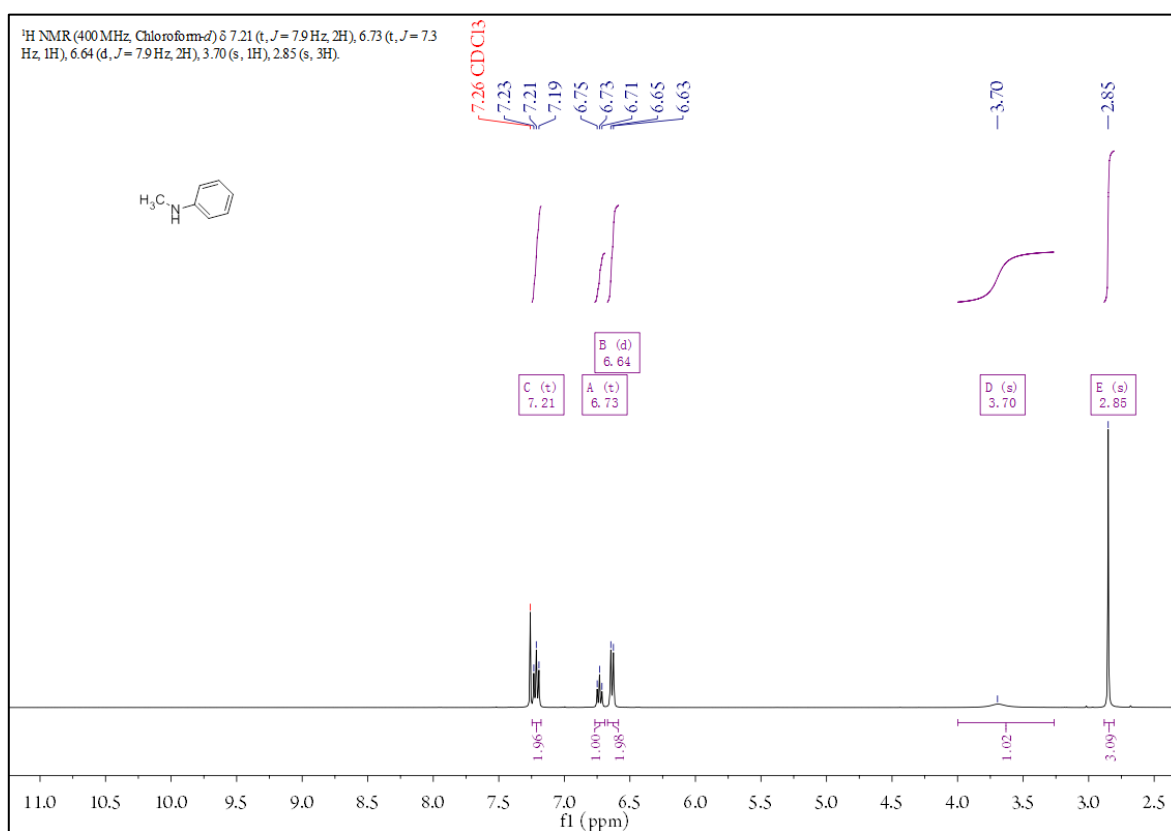
Scheme S35. $^1\text{H-NMR}$ spectrum of 4am in CDCl_3



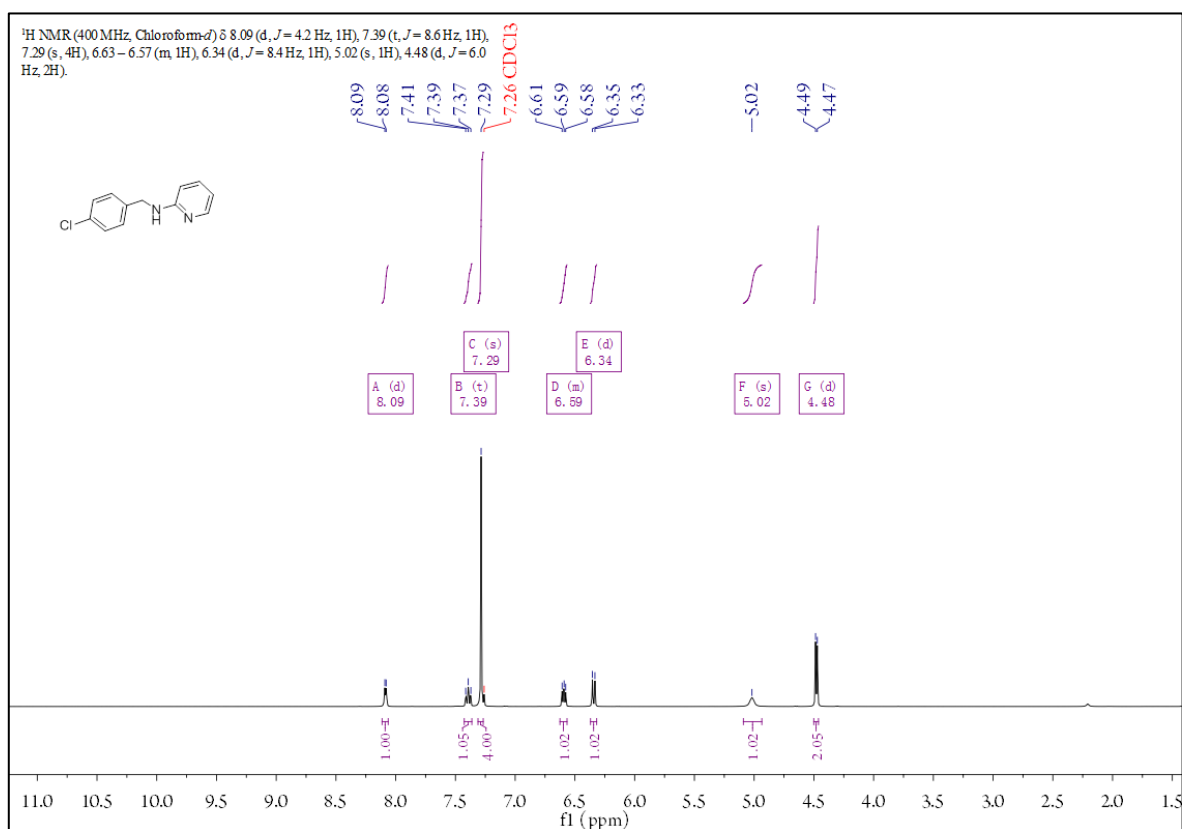
Scheme S36. $^1\text{H-NMR}$ spectrum of 4ao in CDCl_3



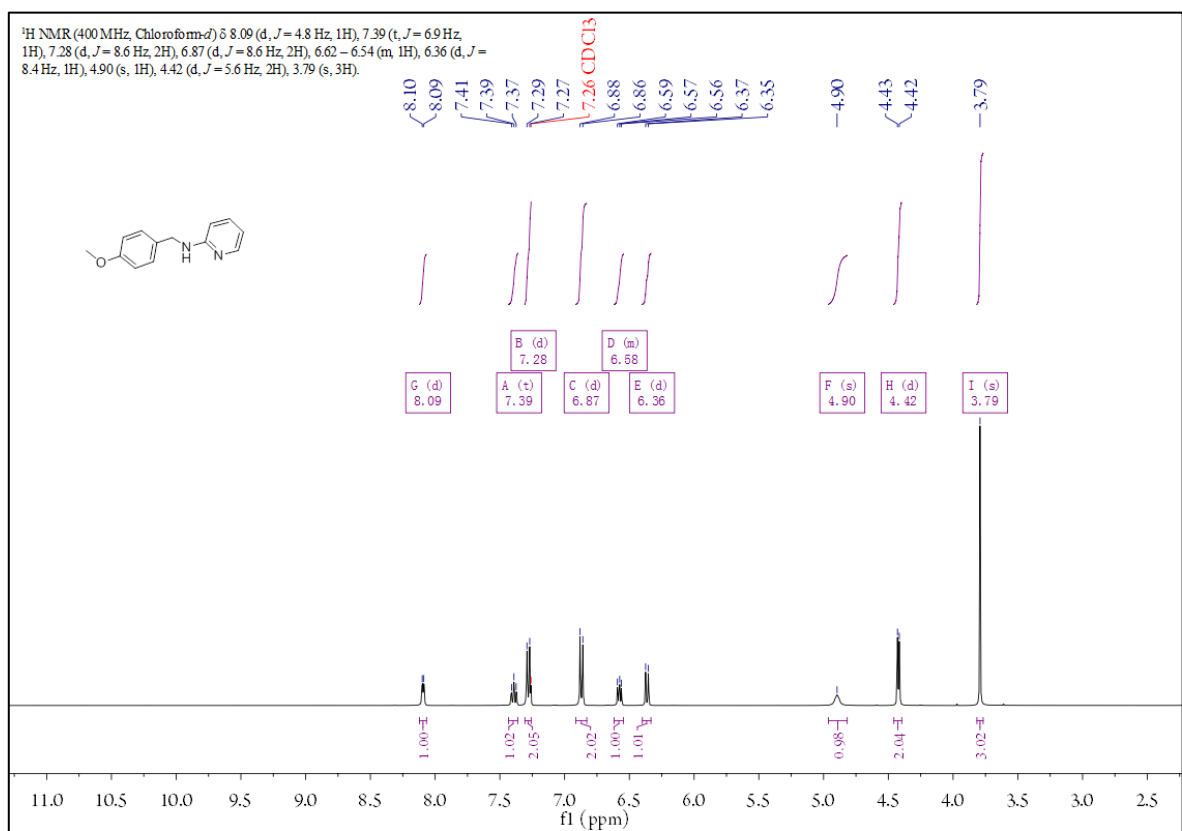
Scheme S37. $^1\text{H-NMR}$ spectrum of 4ap in CDCl_3



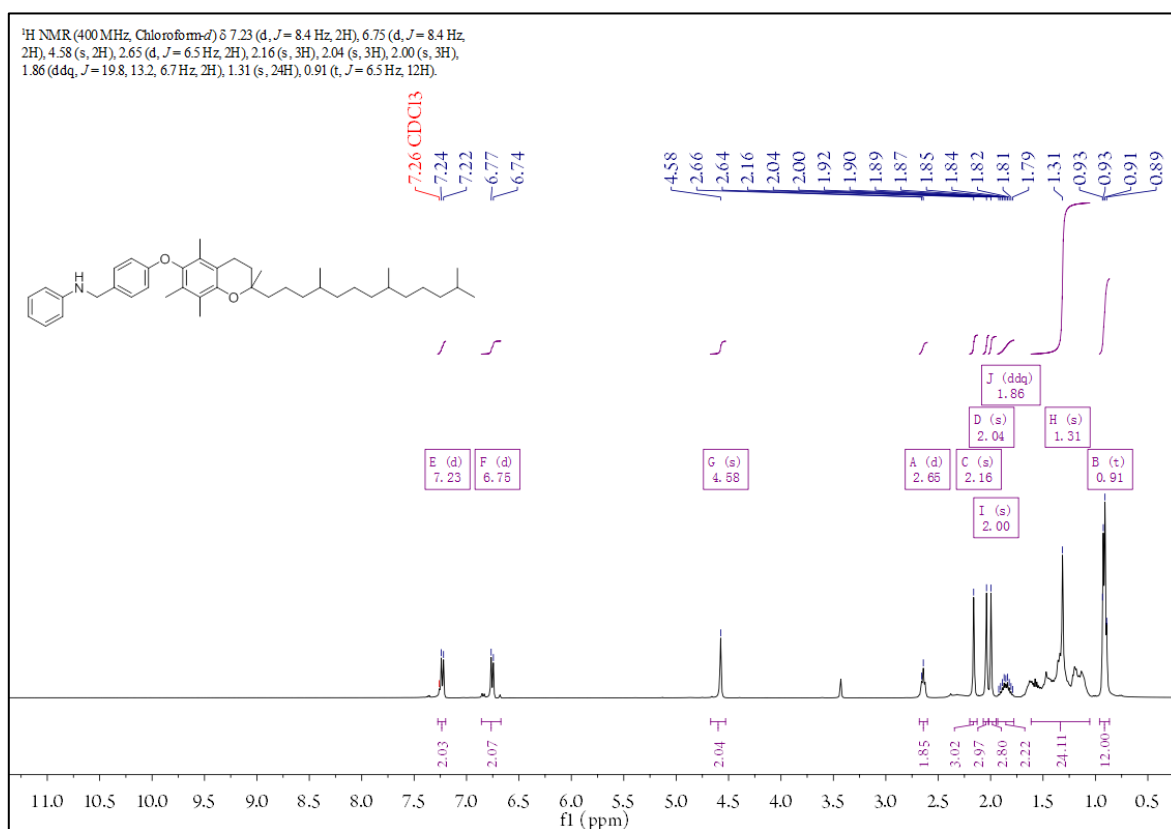
Scheme S38. ¹H-NMR spectrum of 4sb in CDCl₃



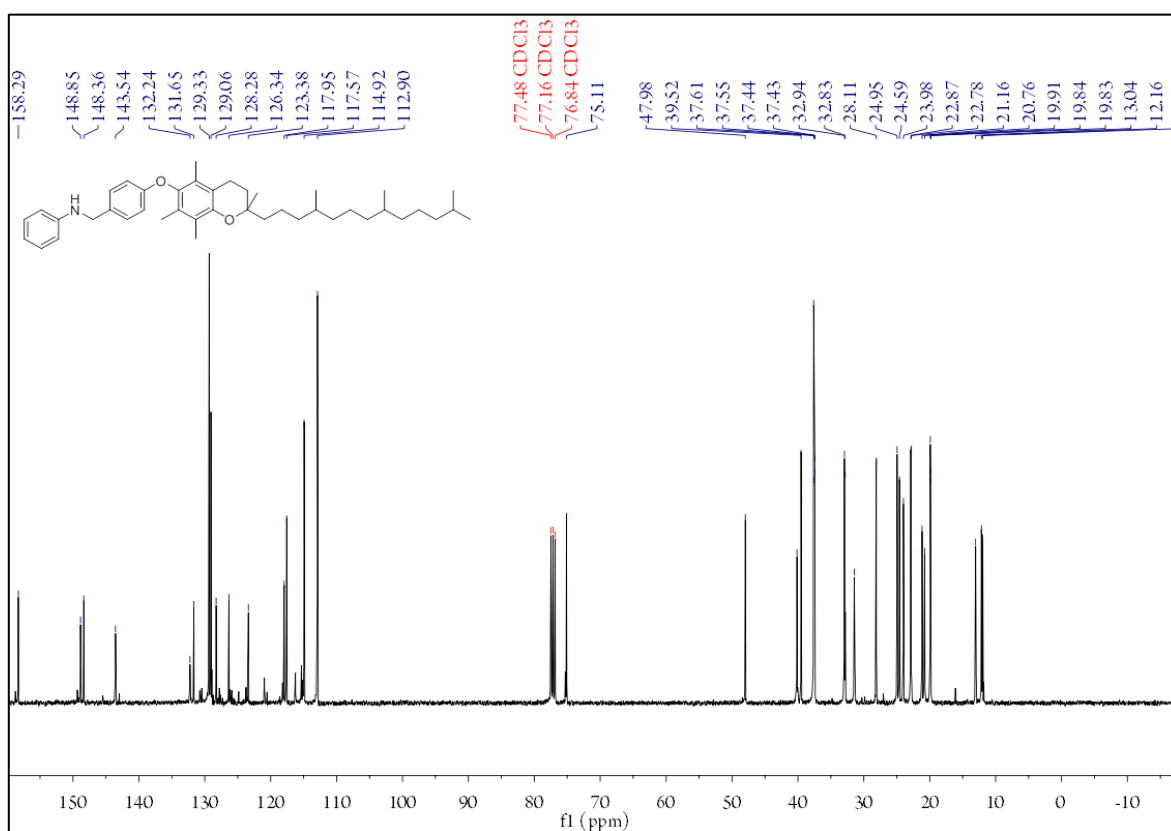
Scheme S39. ¹H-NMR spectrum of 4sf in CDCl₃



Scheme S40. $^1\text{H-NMR}$ spectrum of 4aq in CDCl_3



Scheme S41. $^{13}\text{C-NMR}$ spectrum of 4aq in CDCl_3



16. The Cartesian Coordinates (xyz) for all Optimized Structures in Gas are Presented.

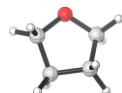
H₂O



0 1

```
O 0.000000 0.000000 0.118453
H 0.000000 0.754537 -0.473811
H 0.000000 -0.754537 -0.473811
```

THF



0 1

```
C -1.155432 -0.423226 -0.134866
O -0.000130 -1.245988 -0.000258
C 1.155242 -0.423506 0.135194
C 0.724845 0.986615 -0.235219
C -0.724512 0.986889 0.235067
H -1.518853 -0.463375 -1.175020
H -1.948936 -0.821307 0.508259
H 1.517915 -0.463518 1.175631
H 1.949088 -0.821919 -0.507286
H 1.341364 1.759740 0.230085
H 0.770330 1.128459 -1.321152
H -0.769912 1.129140 1.320950
H -1.340818 1.760050 -0.230459
```

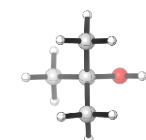
KCl



0 1

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K 0.000000 0.000000 1.289060
Cl 0.000000 0.000000 -1.440715
```

^tBuOH

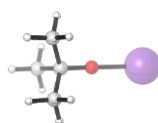


0 1

```
C 0.688636 1.255468 -0.501923
C -0.005438 -0.000005 0.016254
H 0.207909 2.151240 -0.099277
H 1.742860 1.272046 -0.201210
```

```
H 0.659894 1.309907 -1.595226
C 0.691491 -1.253703 -0.502353
C -1.474849 -0.001600 -0.368200
H 0.212943 -2.150709 -0.099855
H 0.662689 -1.307941 -1.595663
H 1.745821 -1.267871 -0.201863
H -1.594899 -0.001159 -1.455328
H -1.972965 -0.886989 0.035758
H -1.975042 0.882183 0.036698
O -0.001040 -0.000219 1.448218
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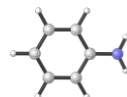
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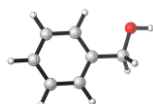


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C 1.167925 1.199324 0.003009
H -0.764696 2.148144 -0.010950
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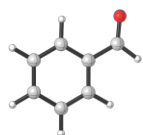
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C	1.352163	1.350222	0.000010
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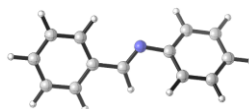


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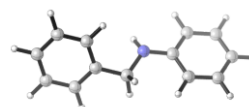
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H	1.674471	-1.857471	0.564712
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H	4.759339	1.858913	-0.581188
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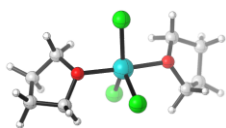


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C	2.429725	-0.983745	0.456512
C	2.649157	1.201630	-0.543915
C	3.817173	-1.094744	0.484070
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C	4.029215	1.073783	-0.518035
H	2.189605	2.104537	-0.941240
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FeCl₃THF₂

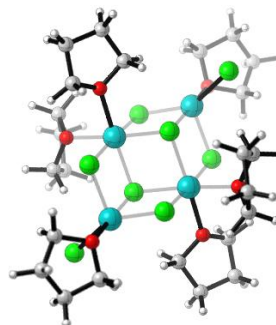


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C	2.780149	-0.035612	-1.071599
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H	2.973925	0.443985	1.928589
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H	4.546818	-1.288289	-1.212850
H	4.764333	0.183042	-0.252073
H	2.895056	0.863398	-1.677626
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C	-3.664230	-1.227020	-0.606797
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Fe₄Cl₈THF₆



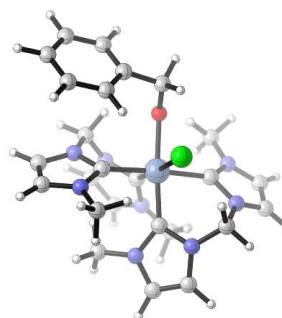
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H	-1.162980	-5.506848	3.348139
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C	-2.705578	-4.161763	2.514338
H	-3.547507	-4.634146	2.003040
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Cr0-ncp-2



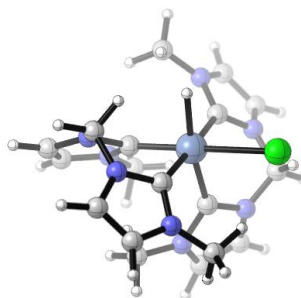
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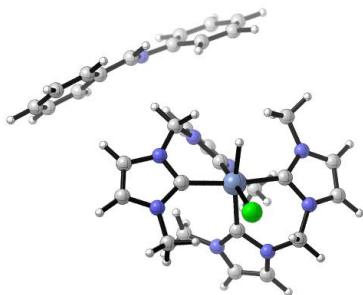


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CrO-ncp-IM3-o



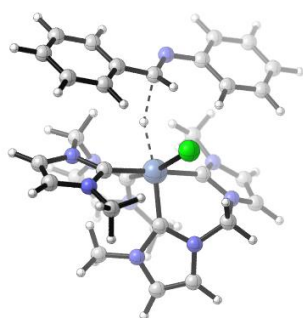
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CrO-ncp-TS2-o



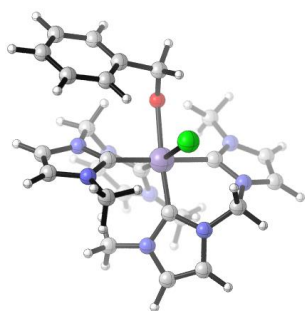
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H	-1.752748	0.832144	1.467935

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C	2.055753	0.953400	1.785364
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H	3.007718	5.477107	1.422149
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H	-5.661218	3.881522	1.152579
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Mn1-ncp-2

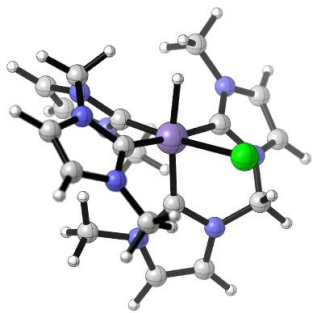


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H	3.998824	0.119931	-2.656997
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H	1.625958	-4.311050	1.034374
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H	1.640023	3.365861	1.981887
H	0.350098	2.237466	1.501110

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Mn1-ncp-3

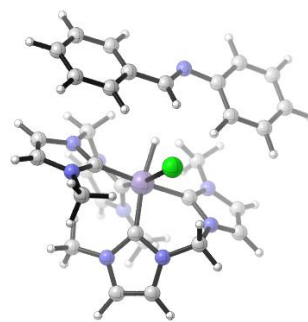


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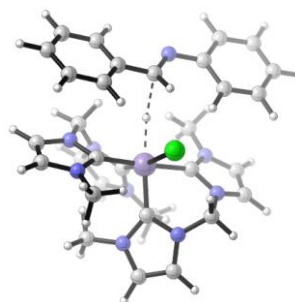
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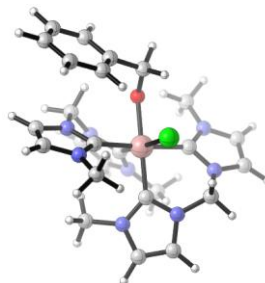


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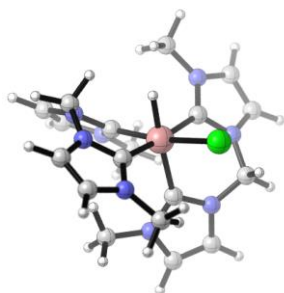
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H	2.002955	-3.617551	0.979660
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C	0.827711	2.739376	1.902913
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Co3-ncp-3

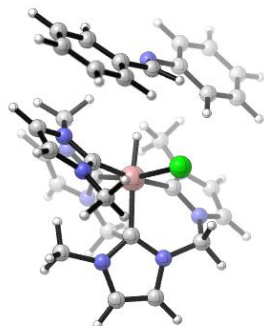


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Co3-ncp-IM3-o



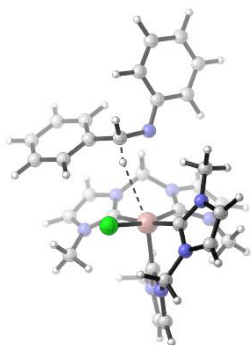
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Co3-ncp-TS2-o

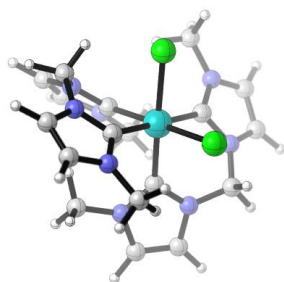


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Fe3-ncp-1

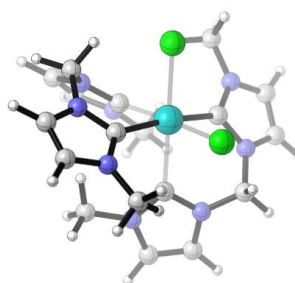


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H	0.281205	-3.220492	3.464668
C	-1.286420	-3.086565	1.902076
H	-2.047921	-3.827548	2.085944
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H	-2.034664	-2.637160	-1.084939
H	-3.245334	-2.776591	0.240090
C	-2.003160	0.199972	-0.629974
C	-4.182438	-0.466739	-0.451046
H	-4.993345	-1.164924	-0.318633
C	-4.176144	0.861123	-0.709686
H	-4.986551	1.559877	-0.842266
C	-2.480063	2.642219	-1.016544
H	-1.524600	2.847828	-0.536310
H	-3.259759	3.275191	-0.587560
H	-2.369079	2.851726	-2.080429
C	1.725892	-1.181163	2.327756
H	1.756810	-1.170936	3.418181
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C	0.259727	1.385318	0.794458
C	0.148343	2.791087	2.573230
H	-0.279294	3.220038	3.465273
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H	2.049415	3.826956	2.085792
C	2.407995	2.198588	-0.155602
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H	3.245586	2.776650	0.238529
C	2.002865	-0.199878	-0.630998

C	4.182283	0.466336	-0.451772
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C	4.175716	-0.861569	-0.710208
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C	2.479298	-2.642228	-1.017712
H	2.367139	-2.851048	-2.081599
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H	3.259467	-3.275455	-0.589982
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Cl	0.208608	1.626044	-2.249023

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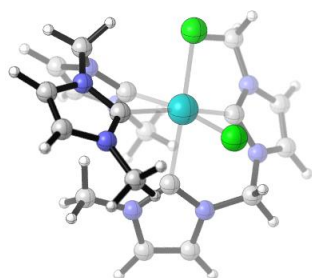


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N	-2.723278	1.586338	-0.629853
C	0.457553	1.317437	0.963293
C	0.592343	2.363488	2.975947
H	0.249352	2.676356	3.949386
C	1.751063	2.613216	2.318511
H	2.618796	3.188062	2.600793
C	2.681032	1.938252	0.082617
H	2.326441	2.487328	-0.797616
H	3.586884	2.388573	0.489721
C	2.009792	-0.321915	-0.671008
C	4.234284	0.017602	-0.350208
H	5.125262	0.576974	-0.114022
C	4.061241	-1.266771	-0.749548
H	4.776070	-2.054869	-0.924285
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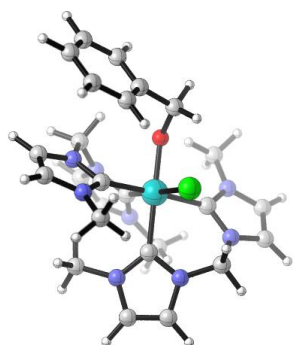
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H	2.068856	-2.791568	-2.421312	N	-2.974071	1.451050	-0.748040
C	-1.493147	1.086009	2.514995	C	0.456517	1.480035	0.810464
H	-1.474292	0.739484	3.550382	C	0.683702	2.613703	2.774161
H	-1.766093	0.256402	1.865145	H	0.378648	2.980165	3.741752
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C	-1.870120	-3.104410	1.665218	H	3.528604	2.615436	0.114092
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H	-3.503569	-2.519904	-0.296071	C	4.302955	-1.157163	-0.503920
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C	-4.074640	1.307855	-0.549766	H	3.183899	-3.519136	-0.633049
H	-4.819846	2.086872	-0.565077	H	2.410613	-2.930163	-2.132583
C	1.373620	-1.730277	2.378432	C	-1.439508	1.356004	2.423201
H	1.737936	-0.860890	1.830958	H	-1.390890	0.983124	3.449076
H	2.089303	-2.549722	2.268906	H	-1.767864	0.553928	1.763503
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H	-1.256481	3.006993	-0.188199	H	-0.379897	-2.979809	3.741863
H	-2.938607	3.615766	-0.252080	C	-1.823962	-2.810765	2.067115
Cl	0.464657	2.037833	-2.160571	H	-2.711296	-3.380558	2.294414
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Fe3-ncps-1



1 6

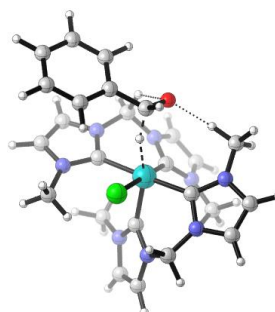
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Fe3-ncp-2

1 2

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N	3.049019	-0.812387	-1.468175
N	2.316879	-2.546222	-0.453045
N	-0.467283	-0.527597	2.507789
N	1.674867	-0.558799	2.495696
N	-2.004434	0.769701	1.228045
N	-1.696217	2.197044	-0.334562
C	1.657488	1.408859	-0.238854
C	2.845018	3.302911	0.193400
H	3.068981	4.232599	0.691486
C	3.481742	2.655568	-0.810031
H	4.372346	2.903311	-1.365091
C	3.099718	0.512116	-2.049316
H	2.389320	0.567376	-2.879920
H	4.118653	0.707505	-2.387870
C	1.987791	-1.259726	-0.739825
C	4.007364	-1.794152	-1.645900
H	4.905599	-1.631732	-2.219933
C	3.540386	-2.891145	-1.003848
H	3.957882	-3.879380	-0.895220
C	1.545992	-3.451442	0.384622
H	0.563023	-3.007950	0.549681
H	2.064299	-3.617978	1.334489
H	1.431093	-4.409651	-0.125712
C	0.849957	2.906322	1.614439
H	1.425687	3.385046	2.408263
H	0.360150	2.019521	2.012936
H	0.085639	3.603944	1.260805
C	0.601683	-0.439449	1.658866
C	1.278119	-0.736898	3.812181
H	1.989657	-0.861134	4.612743
C	-0.074964	-0.710104	3.822054
H	-0.781880	-0.806171	4.630676

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H	-2.137260	-1.288330	1.509659
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H	-3.804938	1.604695	2.086286
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H	-3.394046	3.466662	0.069546
C	3.071217	-0.530811	2.101275
H	3.184487	0.058216	1.192485
H	3.451259	-1.539927	1.915846
H	3.658984	-0.074325	2.899164
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H	-1.737693	2.677176	-2.378064
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C	-1.600184	-2.124413	-1.206873
H	-1.652430	-3.220146	-1.094479
H	-1.203475	-1.900017	-2.203182
C	-2.978832	-1.539121	-1.042984
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C	-5.138566	-1.535326	0.068428
H	-3.620246	-3.038012	0.360250
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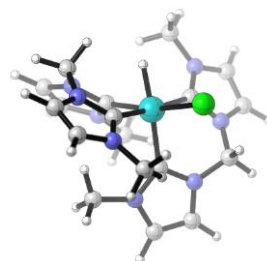
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N	-1.827436	2.098369	-0.153771
C	1.620305	1.429435	-0.174937
C	2.767143	3.317565	0.359018
H	2.981506	4.215851	0.915303
C	3.396215	2.756703	-0.700189
H	4.264873	3.067165	-1.258397
C	3.048901	0.703307	-2.082259
H	2.362981	0.855395	-2.919635
H	4.076799	0.921621	-2.378627
C	1.941957	-1.198056	-0.922344
C	3.956108	-1.610436	-1.925083
H	4.834635	-1.378493	-2.505975
C	3.526191	-2.768545	-1.373392
H	3.962017	-3.754799	-1.364161
C	1.614212	-3.498257	0.029332
H	0.586250	-3.170814	0.218235
H	2.142374	-3.657180	0.976019
H	1.596204	-4.441978	-0.518762
C	0.798626	2.805910	1.774428
H	1.346956	3.376192	2.524950
H	0.427506	1.886914	2.223618
H	-0.052551	3.398526	1.428683
C	0.723559	-0.505511	1.613518
C	1.597194	-0.915790	3.674462
H	2.378450	-1.093503	4.395940
C	0.252222	-0.852353	3.818238
H	-0.377312	-0.973277	4.685183
C	-1.670001	-0.491912	2.259366
H	-1.965964	-1.411717	1.735647
H	-2.218108	-0.370749	3.195354
C	-1.188365	0.990850	0.321553
C	-3.024167	1.487149	1.588052
H	-3.746462	1.345608	2.376017
C	-2.951989	2.399648	0.590668
H	-3.593395	3.230449	0.343684
C	3.229926	-0.683142	1.824936
H	3.313402	0.012780	0.992150
H	3.529059	-1.677961	1.483171
H	3.903979	-0.366953	2.621817
C	-1.419090	2.928453	-1.276021
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H	-0.338446	2.880365	-1.398051
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C	-3.337314	-0.466237	-1.877197
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H	-6.581883	0.044212	-0.997416

Fe3-ncp-3



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N	-1.568948	-1.921436	1.016103
N	0.189432	-1.449050	2.134627
N	-2.867604	-0.601480	-0.483954
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C	0.413642	1.530424	0.437093
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H	0.191534	3.747080	2.857900
C	1.615248	3.307700	1.217280
H	2.425735	4.018555	1.239756
C	2.470043	2.051170	-0.800411
H	1.971170	2.255998	-1.755272
H	3.334207	2.706135	-0.680288
C	1.981261	-0.342720	-0.738246
C	4.201029	0.212610	-0.813361
H	5.054460	0.869910	-0.859699
C	4.110406	-1.138593	-0.798691

H	4.877086	-1.896410	-0.826237	N	1.704141	0.242191	2.231895
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H	1.276162	-2.829246	-0.267168	N	2.901649	0.847585	0.285920
H	2.954020	-3.430232	-0.102766	N	3.117662	-0.148390	-1.590365
H	2.199027	-3.233806	-1.713346	C	0.678056	-2.505919	-0.486078
C	-1.447526	1.660482	2.118494	C	1.429238	-4.651439	-0.547599
H	-1.302260	1.439287	3.179268	H	2.129347	-5.456484	-0.389761
H	-1.793692	0.764403	1.607832	C	0.191305	-4.646093	-1.100526
H	-2.204905	2.442826	2.019068	H	-0.397150	-5.442107	-1.528772
C	-0.404611	-1.213752	0.931250	C	-1.556271	-2.875144	-1.503894
C	-0.574953	-2.283760	2.931369	H	-1.424995	-2.272425	-2.406791
H	-0.261248	-2.588648	3.917160	H	-2.178301	-3.747548	-1.708935
C	-1.690856	-2.585061	2.221545	C	-1.533362	-1.047244	0.141274
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H	-3.445097	-2.441655	0.288597	H	-4.377393	-1.244544	1.777168
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C	-3.990664	1.144548	-1.169653	H	-3.035360	0.912120	2.318697
H	-4.718999	1.880422	-1.470435	C	2.934307	-2.958726	0.491674
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H	2.189934	-1.695778	2.719998	H	3.795741	-3.148204	-0.154087
H	1.344304	-0.324695	3.477285	C	0.815032	-0.612041	1.638950
C	-2.046927	2.618594	-1.731437	C	1.245835	-1.210414	3.796915
H	-2.850268	3.313506	-1.975723	H	1.152824	-1.806368	4.690901
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Fe3-ncp-TS2-o

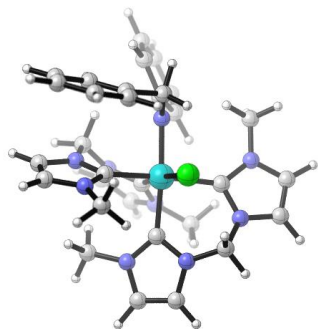


1 2							
Fe	0.331118	-0.540458	-0.270322	C	2.202308	0.073646	-0.602390
N	-0.250863	-3.338409	-1.047664	C	4.185746	1.122201	-0.141231
N	1.705564	-3.346789	-0.175910	H	4.865125	1.746768	0.416784
N	-2.186970	-2.079647	-0.474130	C	4.318828	0.490401	-1.331960
N	-2.397719	-0.678079	1.129019	H	5.152781	0.435617	-2.013565
				C	-0.338093	-2.660154	2.569847
				H	-0.612443	-2.853238	1.536218
				H	-1.248469	-2.477104	3.148996
				H	0.166991	-3.539891	2.976261
				C	2.920570	-0.976388	-2.768926
				H	2.563551	-0.378719	-3.608899
				H	2.167920	-1.734336	-2.556175
				H	3.870241	-1.450972	-3.025420
				Cl	-0.143959	-0.243690	-2.540684

C	-0.758010	2.356332	-0.527506
H	-0.201102	1.137640	0.021340
N	-1.872227	2.650441	0.161842
H	-0.828511	1.949422	-1.542710
C	0.394257	3.286025	-0.374962
C	0.438374	4.246076	0.642611
C	1.463455	3.187161	-1.272893
C	1.548858	5.073830	0.773661
H	-0.415257	4.331272	1.308950
C	2.570670	4.020293	-1.143030
H	1.414691	2.441850	-2.067623
C	2.621053	4.957889	-0.112299
H	1.574876	5.823119	1.560128
H	3.392929	3.941762	-1.849424
H	3.481956	5.613181	-0.013454
C	-3.075047	2.116854	-0.232570
C	-3.282012	1.221236	-1.312814
C	-4.202622	2.497687	0.533890
C	-4.552366	0.740002	-1.589655
H	-2.443562	0.891442	-1.921580
C	-5.469213	2.016026	0.241885
H	-4.037570	3.194568	1.351804
C	-5.653184	1.131172	-0.822289
H	-4.691347	0.055504	-2.423487
H	-6.319737	2.334995	0.837900
H	-6.645133	0.757208	-1.058275

C	-2.812859	-3.207897	1.799018
H	-2.992071	-3.813317	2.672802
C	-3.487605	-3.108238	0.633337
H	-4.374464	-3.604747	0.273712
C	-3.200968	-1.802933	-1.452591
H	-2.522582	-2.265456	-2.177534
H	-4.224453	-2.151522	-1.607936
C	-2.075327	0.423149	-1.420975
C	-4.066675	0.199488	-2.547401
H	-4.972357	-0.297171	-2.856962
C	-3.536460	1.388105	-2.893994
H	-3.892089	2.160467	-3.556718
C	-1.445531	2.611636	-2.554392
H	-1.627410	3.488490	-1.930454
H	-1.621031	2.875188	-3.597898
H	-0.415190	2.293080	-2.441082
C	-0.832852	-2.195505	2.847255
H	-1.334080	-2.572249	3.739106
H	-0.576135	-1.152147	3.009902
H	0.084097	-2.770203	2.693610
C	-0.854967	0.733852	1.417137
C	-1.802605	1.758152	3.223484
H	-2.608763	2.163622	3.813613
C	-0.472501	1.696642	3.461307
H	0.119893	2.039028	4.294560
C	1.492755	0.790524	2.211595
H	1.935859	1.496149	1.501067
H	1.975449	0.922906	3.182016
C	1.033040	-1.144837	0.734846
C	2.655878	-1.410601	2.323484
H	3.304554	-1.111561	3.131523
C	2.572430	-2.563193	1.618784
H	3.135187	-3.480164	1.690896
C	-3.329561	1.092743	1.374519
H	-3.539936	0.080613	1.026585
H	-3.385550	1.770545	0.516815
H	-4.080678	1.384996	2.108323
C	1.190325	-3.471165	-0.222331
H	1.669448	-3.348365	-1.194830
H	0.112210	-3.454743	-0.376122
H	1.493788	-4.414867	0.234445
C	1.761430	0.827594	-1.916857
H	2.173265	1.747894	-2.352109
N	0.805675	1.183570	-0.853484
C	2.900508	-0.096685	-1.556544
C	3.165029	-1.202075	-2.372732
C	3.760394	0.149507	-0.480205

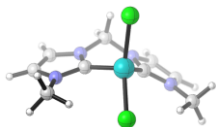
Fe3-ncp-4



1 2			
Fe	-0.483413	-0.219524	-0.230477
N	-2.801034	-2.176608	-0.121108
N	-1.744744	-2.330405	1.723880
N	-3.178233	-0.371022	-1.651261
N	-2.331770	1.508337	-2.216814
N	0.082619	1.061254	2.364210
N	-2.022225	1.155142	1.995932
N	1.711172	-0.567179	1.773558
N	1.579019	-2.391146	0.672380
C	-1.701339	-1.677020	0.515176

C	4.256146	-2.031105	-2.125628
H	2.494946	-1.412311	-3.202207
C	4.850978	-0.678763	-0.228270
H	3.580248	1.003566	0.170477
C	5.104309	-1.773072	-1.051405
H	4.446124	-2.878896	-2.778441
H	5.508437	-0.463944	0.610605
H	5.959959	-2.414618	-0.861001
C	0.935718	2.486330	-0.378248
C	2.157228	3.208962	-0.419054
C	-0.169858	3.168969	0.184847
C	2.267532	4.479714	0.131433
H	3.040503	2.758147	-0.858520
C	-0.052533	4.436718	0.732064
H	-1.141061	2.688444	0.142760
C	1.173110	5.103170	0.726526
H	3.227743	4.986498	0.094299
H	-0.934000	4.919109	1.147385
H	1.266092	6.096330	1.153742
H	1.185058	0.343254	-2.710396
Cl	-0.189213	-1.562412	-2.259400

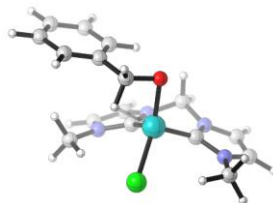
Fe-4coor-1



0 1			
Fe	0.000095	-0.892067	0.534644
N	1.183072	1.607542	-0.168153
N	2.586796	0.033989	-0.574821
N	-1.183576	1.607432	-0.167599
N	-2.586976	0.033650	-0.574541
C	1.322517	0.245121	-0.101801
C	3.208797	1.227606	-0.900895
H	4.212891	1.257985	-1.292399
C	2.324199	2.222312	-0.650216
H	2.399172	3.290442	-0.777301
C	-0.000185	2.259914	0.342575
H	0.000095	2.196868	1.437291
H	-0.000268	3.305206	0.025904
C	-1.322703	0.244957	-0.101534
C	-2.324810	2.222017	-0.649609
H	-2.400084	3.290172	-0.776303
C	-3.209161	1.227165	-0.900564
H	-4.213274	1.257366	-1.292038
C	3.232347	-1.262566	-0.647700

H	2.462399	-2.033925	-0.701405
H	3.864346	-1.427843	0.229681
H	3.847315	-1.313302	-1.548011
C	-3.232143	-1.263028	-0.648021
H	-3.866628	-1.427538	0.227704
H	-2.461940	-2.034319	-0.698827
H	-3.844504	-1.314882	-1.550065
Cl	0.000362	-0.247178	2.683370
Cl	0.000205	-2.551161	-0.991757

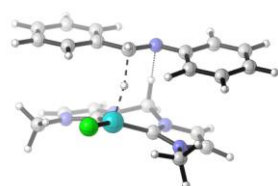
Fe-4coor-2



0 1			
Fe	-0.726092	0.866538	0.163450
N	-2.237206	-1.553170	0.464742
N	-3.576628	0.123434	0.506267
N	-0.142087	-1.827334	-0.594985
N	1.042909	-0.480225	-1.778772
C	-2.246128	-0.181058	0.392472
C	-4.347875	-1.016427	0.659917
H	-5.420500	-0.969584	0.759996
C	-3.507279	-2.078039	0.629038
H	-3.695290	-3.137787	0.696173
C	-0.991674	-2.276373	0.480341
H	-0.486503	-2.103085	1.441086
H	-1.189830	-3.344485	0.363510
C	0.083091	-0.485636	-0.801702
C	0.675263	-2.618647	-1.383394
H	0.637859	-3.696239	-1.360935
C	1.420542	-1.764943	-2.125611
H	2.169687	-1.954718	-2.877638
C	-4.104844	1.472792	0.533808
H	-3.409747	2.128591	0.005412
H	-4.235126	1.817377	1.564323
H	-5.069782	1.497055	0.023967
C	1.668942	0.718186	-2.300054
H	2.621525	0.902608	-1.791124
H	0.988863	1.558794	-2.143687
H	1.846342	0.601885	-3.371187
Cl	-1.397333	2.283575	-1.514928
O	0.085480	0.749573	1.856308
C	1.129959	1.495824	1.371456

H	0.860999	1.946693	0.343032
H	1.306381	2.413247	1.963541
C	2.431698	0.756873	1.151210
C	3.579489	1.447542	0.753149
C	2.494061	-0.626901	1.302519
C	4.762370	0.763837	0.488656
H	3.538998	2.530696	0.640892
C	3.674244	-1.315409	1.034509
H	1.595257	-1.142383	1.631458
C	4.810260	-0.623425	0.621262
H	5.648203	1.312037	0.178332
H	3.708264	-2.396491	1.147972
H	5.731984	-1.159682	0.412291

Fe-4coor-TS2

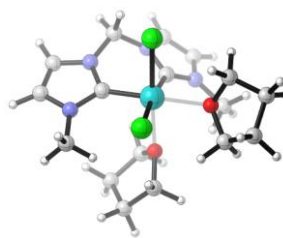


0 1

Fe	0.322404	-1.485375	-0.404964
N	-1.217314	-0.476742	1.853234
N	-2.372248	-1.818057	0.632470
N	1.125849	-0.141890	2.053685
N	2.801907	-1.044894	1.054374
C	-1.111028	-1.280957	0.741761
C	-3.225761	-1.317704	1.597293
H	-4.262653	-1.608596	1.653209
C	-2.502521	-0.468678	2.365702
H	-2.782884	0.129988	3.217873
C	-0.178804	0.449970	2.239803
H	-0.264336	1.363737	1.628529
H	-0.304522	0.700966	3.297586
C	1.439406	-0.892304	0.943742
C	2.247790	0.183453	2.794645
H	2.197834	0.787498	3.686868
C	3.300415	-0.394654	2.167424
H	4.350246	-0.403181	2.414052
C	-2.776475	-2.699633	-0.439508
H	-3.151929	-3.647545	-0.044769
H	-1.908219	-2.892768	-1.076107
H	-3.556284	-2.224269	-1.042752
C	3.605318	-1.794814	0.113298
H	4.477762	-1.206369	-0.180895
H	2.999891	-1.998291	-0.774929
H	3.933998	-2.744741	0.545560

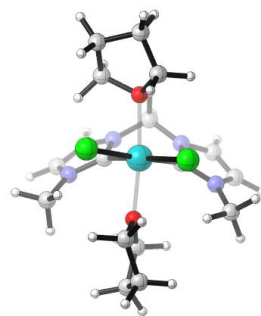
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C	0.105234	1.437699	-1.209546
H	-0.179233	1.103967	-2.222062
H	0.083328	0.009201	-0.760279
C	1.556396	1.697953	-1.050265
C	2.038610	2.586047	-0.085011
C	2.466335	1.007259	-1.859878
C	3.407781	2.782210	0.065411
H	1.318771	3.122786	0.527462
C	3.834006	1.207684	-1.711423
H	2.087101	0.293158	-2.590592
C	4.309551	2.093684	-0.744725
H	3.774654	3.479278	0.814746
H	4.531047	0.668712	-2.348408
H	5.378610	2.252899	-0.628978
N	-0.754752	2.078821	-0.437813
C	-2.105326	1.839213	-0.605944
C	-2.655665	0.803432	-1.394963
C	-2.997693	2.655831	0.119823
C	-4.032855	0.623411	-1.461635
H	-2.000478	0.123899	-1.936542
C	-4.369477	2.471155	0.041900
H	-2.570489	3.445891	0.732845
C	-4.899923	1.452544	-0.751573
H	-4.435642	-0.173517	-2.084401
H	-5.033303	3.124394	0.602958
H	-5.974555	1.306505	-0.814555

Fe-6coor-1a



0 1

Fe	-0.151852	0.001782	-0.479341
N	1.020131	2.506207	0.471876
N	-0.623088	2.005536	1.747223
N	2.520054	1.118726	-0.737546
N	2.665078	-1.005826	-0.957662
C	0.049531	1.549977	0.638083
C	-0.102060	3.201254	2.214589
H	-0.513127	3.708754	3.072901
C	0.938831	3.518221	1.409136
H	1.614121	4.359235	1.416232
C	1.973982	2.450790	-0.612999



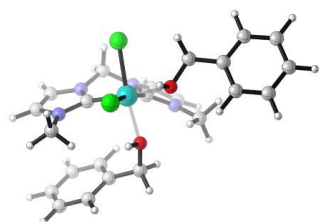
H	1.468649	2.720736	-1.546957
H	2.792058	3.141939	-0.392438
C	1.738295	-0.015557	-0.749151
C	3.855989	0.844870	-0.959650
H	4.607595	1.617466	-0.998243
C	3.945018	-0.497892	-1.099600
H	4.794401	-1.136704	-1.282687
C	-1.723592	1.324395	2.396552
H	-1.602781	0.249003	2.269062
H	-2.684925	1.616019	1.964883
H	-1.713365	1.571328	3.461150
C	2.378771	-2.420513	-1.092198
H	2.219273	-2.686190	-2.139146
H	1.456289	-2.652099	-0.564308
H	3.216931	-2.992180	-0.681375
Cl	-0.681889	-1.915099	-1.798107
Cl	-0.400875	1.407436	-2.348300
O	0.008569	-1.274225	1.315138
C	-0.272662	-2.683844	1.464666
C	0.972593	-0.934655	2.320911
C	0.968238	-3.310813	2.112817
H	-1.160294	-2.790656	2.104617
H	-0.505876	-3.051688	0.460475
C	1.906585	-2.125943	2.372066
H	1.444936	0.001712	2.015912
H	0.454463	-0.780331	3.282862
H	1.430608	-4.060339	1.464838
H	0.701893	-3.815155	3.046177
H	2.653907	-2.034519	1.577734
H	2.440062	-2.202024	3.322837
O	-2.312461	0.048350	-0.116618
C	-2.999981	-1.132880	0.346994
C	-3.155733	0.741278	-1.069245
C	-4.337599	-1.154092	-0.372056
H	-2.381948	-2.002503	0.113383
H	-3.117404	-1.039849	1.439275
C	-4.557996	0.317359	-0.698528
H	-2.934648	1.807230	-0.973144
H	-2.876014	0.424440	-2.080307
H	-5.132341	-1.601356	0.230602
H	-4.244161	-1.730652	-1.298466
H	-4.914307	0.862879	0.185022
H	-5.272210	0.482241	-1.508830

Fe-6coor-1b

O 1			
Fe	-0.086789	0.199182	-0.394547
N	-0.290141	-2.490602	0.712298
N	1.297772	-2.508178	-0.721347
N	-0.894763	-0.769084	2.225874
N	-0.012046	1.165608	2.493107
C	0.355024	-1.669470	-0.184862
C	1.219317	-3.783342	-0.188761
H	1.878770	-4.574820	-0.508145
C	0.220484	-3.776438	0.724308
H	-0.173984	-4.554861	1.358263
C	-1.325272	-1.991669	1.584660
H	-2.235385	-1.812400	1.004846
H	-1.528586	-2.738532	2.355613
C	-0.329680	0.264732	1.510680
C	-0.925967	-0.516295	3.586480
H	-1.347869	-1.208454	4.298260
C	-0.368183	0.706641	3.750443
H	-0.198103	1.291499	4.640627
C	2.304077	-2.147136	-1.703725
H	2.350554	-1.062571	-1.775951
H	2.030630	-2.524289	-2.691124
H	3.266677	-2.569259	-1.395856
C	0.685536	2.418711	2.272857
H	0.221747	3.204009	2.873742
H	0.591412	2.678417	1.215373
H	1.738744	2.326777	2.563935
Cl	-0.733802	2.503704	-0.735656
Cl	0.288330	0.005130	-2.770015
O	1.882041	0.809915	-0.214313
C	2.449955	1.878898	-1.013728
C	2.853384	0.276174	0.694486
C	3.937133	1.617506	-0.938940
H	1.986197	1.800466	-1.999553
H	2.165881	2.838749	-0.562328
C	4.098151	1.127508	0.498019
H	2.444616	0.308378	1.712759
H	3.025556	-0.778891	0.439117
H	4.533324	2.505498	-1.160948

H	4.222718	0.831630	-1.648485
H	4.090733	1.980733	1.186546
H	5.018863	0.566102	0.675011
O	-2.178613	-0.179070	-0.597421
C	-2.703588	-0.104639	-1.958457
C	-3.069823	0.576393	0.276330
C	-4.181443	0.133952	-1.769456
H	-2.209703	0.730923	-2.465102
H	-2.417222	-1.032824	-2.454924
C	-4.164276	1.127177	-0.614793
H	-3.461827	-0.130509	1.024914
H	-2.486539	1.357299	0.769177
H	-4.702532	-0.789565	-1.486472
H	-4.653044	0.527462	-2.673131
H	-5.119653	1.221314	-0.091879
H	-3.864568	2.115607	-0.978551

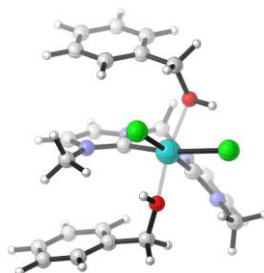
Fe-6coor-1c



O 1			
Fe	0.014318	-0.076325	0.724380
N	0.527360	-2.303325	-1.074510
N	-0.882527	-0.981977	-1.999820
N	2.275101	-1.881416	0.476641
N	2.967728	-0.115550	1.466434
C	-0.161044	-1.140404	-0.840133
C	-0.652232	-2.015380	-2.894382
H	-1.140369	-2.060477	-3.854953
C	0.241695	-2.849362	-2.311219
H	0.688397	-3.768073	-2.657611
C	1.391142	-2.883245	-0.072351
H	0.774269	-3.296438	0.734083
H	1.995403	-3.664782	-0.540846
C	1.839939	-0.644171	0.895913
C	3.596705	-2.117495	0.803928
H	4.097025	-3.042874	0.566096
C	4.030838	-0.997708	1.426659
H	4.998644	-0.738670	1.825828
C	-1.817502	0.096615	-2.254978
H	-1.670950	0.871626	-1.503552
H	-2.851186	-0.258795	-2.190402
H	-1.648928	0.506270	-3.255071

C	3.072864	1.191095	2.085110
H	2.641639	1.183507	3.087196
H	2.526027	1.924620	1.494684
H	4.127593	1.472436	2.119527
Cl	-0.038594	1.632902	2.504438
Cl	-0.622451	-1.827207	2.146961
O	0.235933	1.715679	-0.356953
C	0.983679	2.022451	-1.542206
H	0.529836	1.403801	-2.323271
H	0.798312	3.073669	-1.797147
O	-2.037240	0.556025	0.720327
C	-3.102299	-0.389853	0.793469
H	-2.785356	-1.251316	0.190149
H	-3.191396	-0.779422	1.813808
H	-1.950108	1.042250	1.565374
H	0.433384	2.313600	0.392328
C	-4.404933	0.167553	0.288775
C	-5.548411	-0.637537	0.330281
C	-4.507928	1.455424	-0.238790
C	-6.766246	-0.166635	-0.146042
H	-5.478643	-1.641903	0.744642
C	-5.729525	1.929167	-0.713951
H	-3.621862	2.083480	-0.268303
C	-6.861367	1.121293	-0.671301
H	-7.645374	-0.804192	-0.104141
H	-5.795550	2.936456	-1.117205
H	-7.813419	1.491974	-1.040769
C	2.454029	1.747184	-1.460329
C	2.956006	0.491747	-1.817510
C	3.342990	2.734603	-1.029859
C	4.317779	0.224997	-1.733363
H	2.262867	-0.278438	-2.153979
C	4.707622	2.470786	-0.941859
H	2.960175	3.718604	-0.762262
C	5.195400	1.214503	-1.291883
H	4.696450	-0.755716	-2.008127
H	5.389896	3.247273	-0.607137
H	6.260340	1.007644	-1.228646

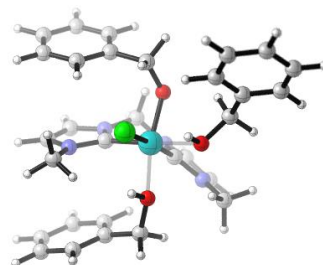
Fe-6coor-1d



O 1
 Fe 0.039575 -1.047563 -0.677382
 N -0.123129 -1.418538 2.199542
 N 1.419287 -2.708189 1.462230
 N -0.807612 0.727471 1.458630
 N -0.066397 1.977764 -0.108795
 C 0.493911 -1.794914 1.031808
 C 1.364604 -2.886617 2.834163
 H 2.016398 -3.577131 3.345528
 C 0.392827 -2.069505 3.305386
 H 0.023214 -1.902833 4.304893
 C -1.190417 -0.445247 2.207946
 H -2.092687 -0.883355 1.771031
 H -1.391521 -0.150147 3.240525
 C -0.257896 0.656418 0.195545
 C -0.954252 2.026519 1.904509
 H -1.396760 2.266186 2.858606
 C -0.484771 2.813328 0.909146
 H -0.404756 3.886348 0.831339
 C 2.318603 -3.465012 0.609729
 H 2.246520 -3.080916 -0.406320
 H 2.018732 -4.514921 0.584941
 H 3.340948 -3.385674 0.993655
 C 0.544051 2.505043 -1.311360
 H -0.218053 2.913931 -1.981430
 H 1.046798 1.701045 -1.840536
 H 1.259962 3.284239 -1.033568
 Cl -0.353244 -0.152354 -2.886192
 O -1.947156 -1.691315 -0.370445
 C -3.029224 -1.168961 -1.178988
 H -2.675643 -1.027051 -2.205310
 H -3.829450 -1.920253 -1.169299
 C -3.510873 0.114213 -0.580413
 C -3.120231 1.341043 -1.123692
 C -4.344750 0.102465 0.542556
 C -3.562121 2.532929 -0.554940
 H -2.453109 1.336921 -1.984949
 C -4.782938 1.293608 1.115070
 H -4.659691 -0.853604 0.959321
 C -4.394007 2.512592 0.562497
 H -3.254355 3.483056 -0.986199
 H -5.440549 1.271927 1.980381
 H -4.742485 3.444380 1.000644
 H -1.673576 -2.557625 -0.766308
 O 1.991682 -0.817852 -1.315280
 C 3.231300 -0.448384 -0.703216
 H 3.322258 -1.117378 0.157555

H 4.040593 -0.693239 -1.402462
 H 1.850484 -0.428341 -2.199441
 C 3.339918 0.976531 -0.249448
 C 2.806164 1.364311 0.983226
 C 3.995301 1.929849 -1.033274
 C 2.912446 2.681889 1.416952
 H 2.296034 0.621007 1.596310
 C 4.111033 3.247832 -0.600010
 H 4.424342 1.630838 -1.988186
 C 3.566485 3.625812 0.625747
 H 2.488953 2.971813 2.374848
 H 4.629126 3.978117 -1.215131
 H 3.660136 4.652497 0.969088
 Cl 0.033065 -3.304345 -1.656554

Fe-6coor-2-1

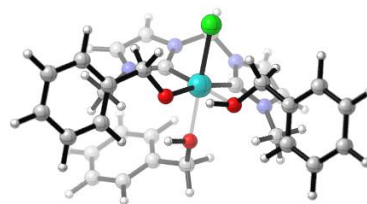


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 Fe -0.277901 -0.420612 -0.099148
 N 0.818832 -0.616130 2.564367
 N -0.125566 -2.483456 2.102333
 N 1.934256 0.929656 1.156955
 N 2.325807 0.920767 -0.946751
 C 0.122570 -1.243926 1.563599
 C 0.393548 -2.600955 3.383065
 H 0.288666 -3.503607 3.963960
 C 0.993934 -1.421370 3.673156
 H 1.514123 -1.088016 4.557581
 C 1.260889 0.754454 2.421506
 H 0.386680 1.411524 2.454873
 H 1.962117 0.984842 3.228253
 C 1.395130 0.493980 -0.032924
 C 3.117532 1.620525 0.983383
 H 3.656481 2.063691 1.805874
 C 3.359566 1.615576 -0.347374
 H 4.170417 2.035075 -0.921789
 C -0.881386 -3.530820 1.448092
 H -1.129881 -3.200301 0.439601
 H -1.809434 -3.729906 1.993088
 H -0.297707 -4.456298 1.410997
 C 2.231486 0.768692 -2.381220

H	1.647997	1.581443	-2.823664
H	1.728191	-0.166276	-2.619274
H	3.239999	0.753021	-2.801205
Cl	-0.959152	0.271577	-2.378538
O	0.255414	-2.128694	-1.276320
C	1.318053	-3.086655	-1.184044
H	1.116890	-3.634422	-0.257946
H	1.218107	-3.794798	-2.016499
O	-2.226376	-1.375221	-0.267148
C	-3.272112	-1.025128	0.663518
H	-3.443685	-1.909563	1.290320
H	-2.870073	-0.211128	1.284432
H	-2.412523	-0.970531	-1.135696
H	0.179662	-1.734327	-2.164938
C	-4.541073	-0.609796	-0.011554
C	-5.767579	-1.162070	0.364228
C	-4.519893	0.371706	-1.010349
C	-6.951602	-0.740895	-0.234853
H	-5.790988	-1.930653	1.134866
C	-5.700946	0.782151	-1.619151
H	-3.569558	0.809648	-1.316423
C	-6.920663	0.231244	-1.230897
H	-7.897865	-1.180554	0.069350
H	-5.667964	1.540701	-2.396327
H	-7.842545	0.556313	-1.705326
C	2.702398	-2.512760	-1.142817
C	3.247003	-2.074755	0.069024
C	3.472019	-2.417410	-2.303851
C	4.528782	-1.539141	0.115000
H	2.648694	-2.149768	0.975845
C	4.757130	-1.881362	-2.262279
H	3.058719	-2.768420	-3.248512
C	5.285202	-1.439323	-1.052281
H	4.938585	-1.195040	1.060706
H	5.347483	-1.815626	-3.172178
H	6.288813	-1.024106	-1.015955
O	-1.176472	0.973757	0.935435
C	-1.537817	2.188916	0.360022
H	-1.911360	2.081015	-0.674381
H	-2.373999	2.613966	0.950264
C	-0.412469	3.197302	0.345001
C	-0.033518	3.866973	1.513880
C	0.303953	3.453896	-0.827340
C	1.029234	4.767101	1.515107
H	-0.599228	3.687185	2.428492
C	1.368224	4.353058	-0.833186
H	0.008864	2.927533	-1.735481

C	1.733102	5.014999	0.337373
H	1.298342	5.291377	2.429651
H	1.913282	4.541707	-1.756700
H	2.557696	5.723585	0.332096

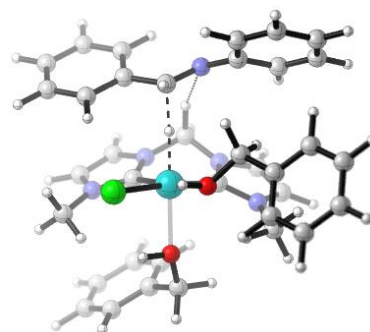
Fe-6coor-2-2



O	1		
Fe	0.279714	-0.405795	-0.473627
N	0.454876	-3.232825	-1.172419
N	1.768854	-2.846940	0.474553
N	-1.568143	-2.179674	-1.836468
N	-2.689762	-0.531865	-1.052623
C	0.893978	-2.207360	-0.371454
C	1.870908	-4.199127	0.187536
H	2.517912	-4.857351	0.745560
C	1.038755	-4.444780	-0.852921
H	0.818669	-5.355897	-1.387021
C	-0.450506	-2.987648	-2.270607
H	0.085207	-2.456132	-3.065554
H	-0.831601	-3.945629	-2.634475
C	-1.412759	-1.028126	-1.094832
C	-2.874741	-2.371505	-2.245370
H	-3.173677	-3.209417	-2.855581
C	-3.581908	-1.332663	-1.742138
H	-4.632658	-1.095656	-1.799409
C	2.527866	-2.186228	1.516966
H	2.153383	-1.168437	1.624942
H	3.589686	-2.139294	1.255095
H	2.422184	-2.728621	2.461416
C	-3.114544	0.627889	-0.296754
H	-3.527476	1.390915	-0.963381
H	-2.243024	1.050427	0.203085
H	-3.871098	0.336098	0.437997
Cl	0.952675	-0.138239	-2.715592
O	-0.079251	-0.188324	1.569220
C	-0.667974	-1.073257	2.527424
H	-0.163127	-2.030575	2.362059
H	-0.398624	-0.717748	3.531579
O	2.107825	0.552786	0.162472
C	3.268709	0.596389	-0.656621
H	3.380175	-0.398205	-1.109309
H	3.111247	1.273302	-1.505384

H	1.542702	1.361144	0.040556
H	-0.526621	0.678880	1.503869
C	4.505020	0.965596	0.117418
C	5.723894	1.076013	-0.560470
C	4.480611	1.185126	1.494940
C	6.890785	1.397808	0.122392
H	5.752132	0.909457	-1.636123
C	5.650017	1.509228	2.180621
H	3.533372	1.104154	2.020504
C	6.858216	1.615840	1.499135
H	7.828681	1.481932	-0.420390
H	5.614692	1.681564	3.253502
H	7.769101	1.869837	2.034222
C	-2.152958	-1.235381	2.414882
C	-2.701745	-2.230228	1.601213
C	-3.011034	-0.396596	3.132708
C	-4.081616	-2.379728	1.501311
H	-2.034357	-2.880948	1.037310
C	-4.391733	-0.545764	3.039774
H	-2.588646	0.373617	3.776567
C	-4.928506	-1.538742	2.222184
H	-4.495770	-3.154735	0.862189
H	-5.048176	0.107930	3.606882
H	-6.005783	-1.661281	2.151907
O	-0.149928	1.553014	-0.214198
C	-0.615451	2.354478	-1.244257
H	0.213382	2.730370	-1.874652
H	-1.235197	1.772693	-1.956819
C	-1.431029	3.534680	-0.768553
C	-1.646421	3.780179	0.587895
C	-2.011463	4.402758	-1.700696
C	-2.420241	4.861874	1.005766
H	-1.191757	3.106831	1.310995
C	-2.783750	5.482679	-1.289461
H	-1.851000	4.221664	-2.762954
C	-2.992899	5.717314	0.069828
H	-2.574336	5.038489	2.067970
H	-3.226259	6.145026	-2.029639
H	-3.596199	6.561332	0.393454

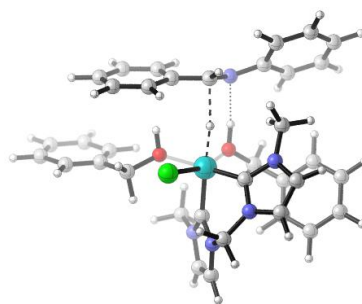
Fe-6coor-TS2-1



O 1			
Fe	0.363399	-0.459391	-0.496395
N	0.451509	0.194762	2.330253
N	-0.843942	-1.491280	2.049264
N	2.327110	0.957305	1.089359
N	3.311738	0.221701	-0.664293
C	-0.059873	-0.606727	1.337188
C	-0.824811	-1.218664	3.407704
H	-1.389659	-1.803266	4.116467
C	-0.004045	-0.155766	3.586046
H	0.286071	0.376771	4.478237
C	1.286600	1.331207	2.019295
H	0.655599	2.132957	1.608893
H	1.756456	1.682071	2.942350
C	2.083935	0.212227	-0.046219
C	3.620571	1.439407	1.142037
H	3.971139	2.070366	1.943525
C	4.239115	0.972954	0.033422
H	5.251662	1.094991	-0.317556
C	-1.628157	-2.561675	1.467749
H	-1.316632	-2.703543	0.433156
H	-2.696223	-2.318859	1.478495
H	-1.474476	-3.485734	2.032984
C	3.621850	-0.405986	-1.929242
H	3.326762	0.231054	-2.767292
H	3.075780	-1.343988	-2.017864
H	4.694349	-0.610607	-1.965757
Cl	0.590071	-0.543894	-2.939524
C	-0.528198	2.521368	-0.561893
H	-1.120789	2.288877	-1.466798
H	-0.099929	1.114439	-0.453629
C	0.792099	3.154045	-0.859413
C	1.295136	4.163013	-0.031598
C	1.527266	2.770269	-1.986255
C	2.513428	4.772493	-0.320568
H	0.699159	4.468184	0.824797
C	2.740997	3.384090	-2.275846
H	1.148731	1.966719	-2.616439
C	3.240532	4.385502	-1.443544

H	2.889087	5.562352	0.325641
H	3.300610	3.079569	-3.157627
H	4.187752	4.866740	-1.674246
O	0.733281	-2.572461	-0.801792
C	1.438240	-3.509321	0.025437
H	0.832360	-3.579528	0.934725
H	1.419386	-4.490788	-0.466242
O	-1.571358	-1.052972	-1.140953
C	-2.792401	-0.434480	-0.747649
H	-2.664233	-0.134891	0.301608
H	-2.943603	0.505360	-1.298127
H	-1.410375	-0.936583	-2.097739
H	1.094557	-2.533579	-1.704970
C	-3.976728	-1.350372	-0.902299
C	-5.241058	-0.901959	-0.506445
C	-3.845900	-2.640758	-1.417775
C	-6.352221	-1.728120	-0.630073
H	-5.345296	0.102136	-0.097701
C	-4.961362	-3.466985	-1.542168
H	-2.862895	-2.993839	-1.717923
C	-6.217147	-3.014665	-1.149933
H	-7.328911	-1.366455	-0.319044
H	-4.845937	-4.468500	-1.948555
H	-7.086371	-3.659222	-1.247785
C	2.841903	-3.115779	0.372174
C	3.094393	-2.328403	1.500069
C	3.915168	-3.524195	-0.422334
C	4.392308	-1.946819	1.819412
H	2.257649	-2.008852	2.119471
C	5.217096	-3.142009	-0.107359
H	3.727342	-4.149164	-1.294608
C	5.455805	-2.350887	1.013212
H	4.575899	-1.328802	2.694066
H	6.044465	-3.467729	-0.731911
H	6.470907	-2.054465	1.263489
N	-1.129436	2.866944	0.570647
C	-2.490132	2.692750	0.698114
C	-3.006903	2.263916	1.938859
C	-3.416558	2.986952	-0.327114
C	-4.373536	2.119591	2.137945
H	-2.299379	2.046489	2.736553
C	-4.783245	2.854756	-0.116082
H	-3.046650	3.358383	-1.280321
C	-5.275089	2.417733	1.114848
H	-4.742416	1.780052	3.103165
H	-5.475177	3.104680	-0.917466
H	-6.345073	2.321788	1.277298

Fe-6coor-TS2-2

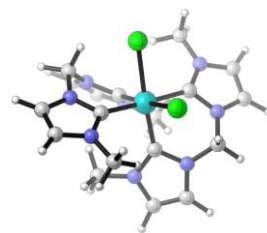


O	1		
Fe	0.045285	-0.659546	-0.592179
N	-0.402086	-3.555276	-0.438871
N	0.717113	-2.987490	1.293957
N	-2.001011	-2.364762	-1.728673
N	-2.804602	-0.393999	-1.519907
C	0.195363	-2.457969	0.133914
C	0.438884	-4.340363	1.423424
H	0.773180	-4.919473	2.269906
C	-0.276001	-4.696970	0.328339
H	-0.684079	-5.649401	0.026840
C	-1.063253	-3.460714	-1.722623
H	-0.307148	-3.290891	-2.497926
H	-1.605229	-4.391940	-1.908031
C	-1.663230	-1.110478	-1.272089
C	-3.276523	-2.409088	-2.262197
H	-3.704495	-3.311824	-2.668927
C	-3.781748	-1.160352	-2.128952
H	-4.748012	-0.755899	-2.386305
C	-2.934463	1.014785	-1.240030
H	-2.593711	1.621401	-2.086078
H	-2.314870	1.251510	-0.377868
H	-3.975060	1.258747	-1.009251
C	1.461681	-2.226062	2.273643
H	1.067624	-2.415004	3.277394
H	1.365756	-1.167691	2.028341
H	2.523620	-2.495683	2.259997
Cl	1.014415	-1.174245	-2.704355
C	0.071646	2.772555	-0.766832
H	-0.459798	2.865053	-1.723125
H	-0.152966	0.877305	-1.175079
C	1.536401	2.708073	-0.867741
C	2.339869	3.190126	0.176172
C	2.150316	2.177286	-2.015161
C	3.727199	3.137274	0.077496
H	1.849403	3.597973	1.055381
C	3.536464	2.122690	-2.104602

H	1.528530	1.730902	-2.788393
C	4.329178	2.603597	-1.059962
H	4.342623	3.499355	0.896701
H	3.998617	1.677239	-2.981655
H	5.412257	2.538282	-1.121259
O	-0.466305	0.292313	1.221855
C	-1.295962	-0.106233	2.324337
H	-0.706962	-0.818174	2.915696
H	-1.473134	0.775591	2.952368
O	2.020840	-0.160789	0.098471
C	3.149429	-0.923045	-0.338462
H	2.883610	-1.968417	-0.132765
H	3.249525	-0.851330	-1.428183
H	2.142947	0.744402	-0.228511
H	-0.506649	1.267010	1.082658
C	4.414070	-0.518871	0.362729
C	5.646300	-0.749021	-0.255432
C	4.394937	0.090793	1.619280
C	6.834722	-0.386356	0.370212
H	5.666915	-1.204051	-1.244275
C	5.582617	0.463012	2.243144
H	3.436640	0.300434	2.088431
C	6.806200	0.224744	1.622302
H	7.784486	-0.567996	-0.125906
H	5.552129	0.947105	3.216072
H	7.732537	0.518671	2.108118
C	-2.595821	-0.740289	1.923421
C	-2.672243	-2.122957	1.731555
C	-3.744378	0.030202	1.728863
C	-3.859668	-2.718959	1.320953
H	-1.790227	-2.736016	1.906316
C	-4.936909	-0.563475	1.324472
H	-3.697574	1.107739	1.878318
C	-4.994962	-1.938764	1.112506
H	-3.897036	-3.794592	1.162908
H	-5.821588	0.050579	1.174573
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N	-0.500915	3.056351	0.379526
C	-1.797068	3.568673	0.400286
C	-2.526855	3.450086	1.596742
C	-2.406801	4.250588	-0.671664
C	-3.824639	3.933729	1.702917
H	-2.042567	2.967672	2.444046
C	-3.704477	4.733659	-0.560039
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C	-4.429476	4.570171	0.620103
H	-4.365044	3.817738	2.639402

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Fe2-ncp-1

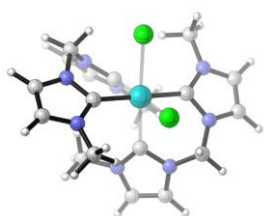


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N	-2.843362	-0.819820	-0.405422
N	-2.810181	1.288301	-0.740450
N	1.347276	2.219034	0.791937
N	-0.424072	1.736680	1.900480
N	2.843347	0.819868	-0.405197
N	2.810305	-1.288239	-0.740337
C	-0.262740	-1.367308	0.759975
C	-0.202397	-2.774905	2.572867
H	0.204468	-3.200255	3.476783
C	-1.323714	-3.074598	1.876954
H	-2.090832	-3.813317	2.048800
C	-2.389289	-2.179184	-0.213511
H	-1.980472	-2.550911	-1.161180
H	-3.229954	-2.784985	0.134157
C	-1.968335	0.218634	-0.602828
C	-4.165539	-0.419632	-0.439658
H	-4.986634	-1.110374	-0.328549
C	-4.141258	0.916850	-0.657326
H	-4.942164	1.630999	-0.767244
C	-2.405969	2.670196	-0.919345
H	-1.382257	2.791644	-0.569825
H	-3.089662	3.312137	-0.354199
H	-2.417080	2.943353	-1.975666
C	1.665479	-1.154340	2.360203
H	1.658040	-1.097729	3.451911
H	1.768204	-0.151204	1.949295
H	2.528817	-1.748840	2.041620
C	0.262642	1.367197	0.760049
C	0.202141	2.774716	2.572989
H	-0.204796	3.200022	3.476892
C	1.323491	3.074478	1.877155
H	2.090573	3.813218	2.049072
C	2.389159	2.179200	-0.213340

H	1.980328	2.550873	-1.161028
H	3.229766	2.785077	0.134333
C	1.968392	-0.218630	-0.602668
C	4.165550	0.419758	-0.439355
H	4.986599	1.110546	-0.328189
C	4.141356	-0.916720	-0.657067
H	4.942310	-1.630816	-0.766970
C	-1.665779	1.154227	2.360021
H	-1.768497	0.151120	1.949041
H	-2.529049	1.748784	2.041357
H	-1.658483	1.097555	3.451726
C	2.406188	-2.670143	-0.919374
H	2.417596	-2.943278	-1.975699
H	1.382383	-2.791627	-0.570141
H	3.089751	-3.312081	-0.354067
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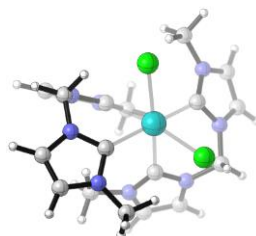


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N	2.937114	0.466856	-0.454152
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N	-1.740615	-2.042623	0.864689
N	0.015567	-1.789039	2.046775
N	-2.937153	-0.466861	-0.453870
N	-2.621341	1.620926	-0.792077
C	0.514944	1.440523	0.834986
C	0.847776	2.579630	2.789133
H	0.592854	2.959832	3.766365
C	1.966772	2.736110	2.037607
H	2.879378	3.279407	2.228918
C	2.679380	1.871863	-0.232552
H	2.226788	2.289969	-1.143351
H	3.617066	2.367673	0.026653
C	1.929427	-0.443779	-0.686671
C	4.188878	-0.119470	-0.431117
H	5.093834	0.449052	-0.284743
C	3.985459	-1.439441	-0.653610

H	4.681883	-2.258938	-0.736266
C	2.028420	-2.929549	-0.992456
H	1.023713	-2.931433	-0.570036
H	2.658904	-3.675620	-0.499269
H	1.926132	-3.153026	-2.055071
C	-1.335031	1.399313	2.496903
H	-1.279705	0.938064	3.487704
H	-1.738889	0.677313	1.786879
H	-2.001936	2.266083	2.544220
C	-0.514871	-1.440510	0.835067
C	-0.847534	-2.579545	2.789282
H	-0.592528	-2.959713	3.766505
C	-1.966594	-2.736053	2.037859
H	-2.879185	-3.279342	2.229269
C	-2.679405	-1.871866	-0.232262
H	-2.226897	-2.289995	-1.143092
H	-3.617069	-2.367663	0.027040
C	-1.929483	0.443763	-0.686506
C	-4.188909	0.119478	-0.430726
H	-5.093857	-0.449032	-0.284249
C	-3.985502	1.439441	-0.653282
H	-4.681928	2.258940	-0.735903
C	1.335271	-1.399284	2.496797
H	1.739074	-0.677317	1.786709
H	2.002161	-2.266068	2.544076
H	1.280054	-0.938001	3.487589
C	-2.028472	2.929501	-0.992461
H	-1.926330	3.152907	-2.055106
H	-1.023704	2.931384	-0.570185
H	-2.658863	3.675622	-0.499234
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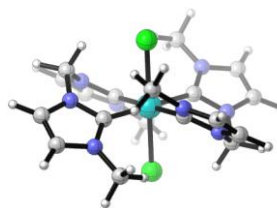


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N	3.092154	0.611500	-0.385272
N	2.997308	-1.481852	-0.762872
N	-1.700008	-2.083938	0.880530

N	0.074626	-1.752175	2.004502
N	-3.092172	-0.611536	-0.384992
N	-2.997331	1.481832	-0.762506
C	0.481372	1.473427	0.790167
C	0.763762	2.504739	2.813040
H	0.481337	2.831918	3.801950
C	1.898534	2.707763	2.097910
H	2.802664	3.245724	2.339069
C	2.674907	1.983670	-0.195949
H	2.196325	2.333881	-1.119733
H	3.545436	2.590263	0.060625
C	2.217884	-0.362964	-0.803582
C	4.349292	0.113183	-0.086935
H	5.165988	0.742478	0.232354
C	4.287981	-1.217210	-0.335527
H	5.042650	-1.985687	-0.268846
C	2.523584	-2.819327	-1.068394
H	1.534239	-2.741393	-1.529208
H	2.465012	-3.417175	-0.151921
H	3.212037	-3.305363	-1.763625
C	-1.390589	1.304567	2.409483
H	-1.330508	0.730242	3.339310
H	-1.787683	0.666987	1.619694
H	-2.062844	2.154937	2.559505
C	-0.481231	-1.473599	0.790164
C	-0.763705	-2.504391	2.813298
H	-0.481296	-2.831365	3.802280
C	-1.898508	-2.707476	2.098235
H	-2.802691	-3.245281	2.339541
C	-2.674901	-1.983716	-0.195711
H	-2.196398	-2.333919	-1.119534
H	-3.545413	-2.590308	0.060917
C	-2.217924	0.362945	-0.803309
C	-4.349281	-0.113220	-0.086542
H	-5.165965	-0.742520	0.232769
C	-4.287982	1.217182	-0.335096
H	-5.042645	1.985659	-0.268338
C	1.390818	-1.304657	2.409371
H	1.787952	-0.667258	1.619455
H	2.062961	-2.155101	2.559483
H	1.330887	-0.730176	3.339111
C	-2.523605	2.819308	-1.068029
H	-3.212060	3.305345	-1.763258
H	-1.534264	2.741364	-1.528858
H	-2.465035	3.417156	-0.151556
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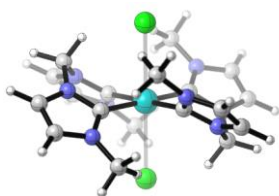
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N	2.679365	1.187788	-0.420771
N	1.567711	2.536018	0.808942
N	2.679246	-1.188028	-0.420788
N	1.567447	-2.536171	0.808887
C	-1.439778	1.343138	-0.147493
C	-2.823461	3.093941	-0.637763
H	-3.100268	4.033006	-1.090706
C	-3.533405	2.237286	0.134286
H	-4.548482	2.278032	0.497191
C	-3.031229	0.000143	1.169518
H	-2.483934	0.000116	2.118159
H	-4.110639	0.000188	1.338755
C	-1.439899	-1.342983	-0.147502
C	-3.533570	-2.236999	0.134363
H	-4.548633	-2.277685	0.497316
C	-2.823735	-3.093662	-0.637778
H	-3.100634	-4.032687	-1.090748
C	-0.540102	-3.157581	-1.620507
H	0.192644	-2.397867	-1.892646
H	-0.991330	-3.547615	-2.535605
H	-0.058688	-3.983133	-1.083385
C	-0.539849	3.157625	-1.620554
H	-0.991044	3.547650	-2.535673
H	0.192847	2.397853	-1.892660
H	-0.058384	3.983167	-1.083461
C	1.439736	1.342983	0.147173
C	2.823960	3.093086	0.638473
H	3.100842	4.032042	1.091597
C	3.533684	2.236639	-0.133976
H	4.548687	2.277399	-0.497087
C	3.031401	-0.000132	-1.169696
H	2.485083	-0.000096	-2.118884
H	4.110939	-0.000182	-1.338136
C	1.439598	-1.343109	0.147144

C	3.533471	-2.236950	-0.133971
H	4.548484	-2.277789	-0.497045
C	2.823627	-3.093383	0.638383
H	3.100396	-4.032397	1.091456
C	0.540228	3.157383	1.620734
H	-0.192169	2.397677	1.893848
H	0.058272	3.982397	1.083282
H	0.991788	3.548258	2.535309
C	0.539889	-3.157461	1.620639
H	0.057945	-3.982482	1.083183
H	-0.192502	-2.397720	1.893667
H	0.991365	-3.548313	2.535266
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Fe2-cpt-1

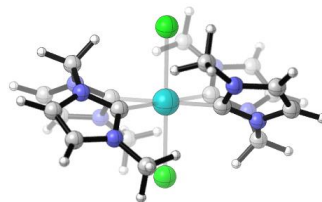


0 3

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N	2.680218	-1.189245	0.423198
N	1.592694	-2.535904	-0.835560
N	2.680156	1.189312	0.423203
N	1.592545	2.535888	-0.835562
C	-1.453371	-1.363579	0.156998
C	-2.854055	-3.078229	0.664156
H	-3.147890	-4.004006	1.132791
C	-3.547172	-2.224477	-0.129135
H	-4.559030	-2.259469	-0.500710
C	-2.999985	0.000005	-1.191359
H	-2.397166	-0.000004	-2.111925
H	-4.069291	0.000019	-1.410808
C	-1.453336	1.363533	0.156993
C	-3.547108	2.224499	-0.129107
H	-4.558967	2.259529	-0.500673
C	-2.853959	3.078218	0.664196
H	-3.147760	4.003994	1.132851
C	-0.562127	3.127470	1.669881
H	0.042326	2.319277	2.093294
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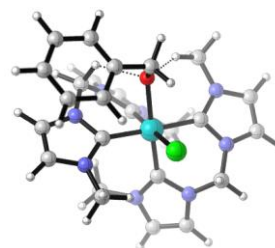
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H	0.042240	-2.319449	2.093324
H	0.062503	-3.818034	1.092661
C	1.453417	-1.363541	-0.156902
C	2.854019	-3.078202	-0.664264
H	3.147790	-4.003962	-1.132970
C	3.547242	-2.224469	0.128955
H	4.559149	-2.259476	0.500395
C	3.000277	0.000042	1.191214
H	2.397661	0.000024	2.111906
H	4.069632	0.000069	1.410433
C	1.453347	1.363531	-0.156892
C	3.547117	2.224586	0.128938
H	4.559024	2.259657	0.500370
C	2.853838	3.078268	-0.664292
H	3.147550	4.004038	-1.133017
C	0.562196	-3.127340	-1.669950
H	-0.042261	-2.319105	-2.093274
H	-0.062622	-3.817786	-1.092751
H	1.039201	-3.677299	-2.482975
C	0.561969	3.127219	-1.669928
H	-0.062928	3.817566	-1.092697
H	-0.042393	2.318909	-2.093253
H	1.038890	3.677246	-2.482957
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Cl	0.191429	0.000038	2.818730

Fe2-cpq-1



0 5

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N	2.018728	-2.534376	-0.699307
N	2.888132	1.189436	0.702388
N	2.018727	2.534377	-0.699301
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C	-3.350936	-2.894533	0.586360



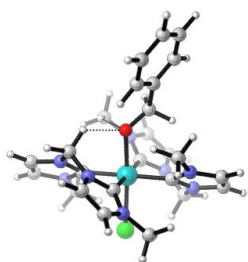
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Fe2-ncp-2

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C	-3.370062	-0.266946	-1.684836
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Fe2-cp-2

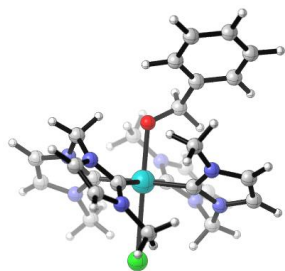


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C	-1.447056	2.029382	3.135222
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H	-1.851853	-0.700962	1.248873
H	-3.142737	0.205111	2.066666
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H	-0.012002	1.640890	-3.792159
H	0.135283	0.281434	-2.639873
H	1.537253	0.777206	-3.643542
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C	3.033691	-2.080503	-2.742836
H	3.893628	-2.161161	-3.389177
C	1.991523	-2.923086	-2.542061
H	1.755974	-3.881823	-2.977199
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C	3.752230	0.129287	-1.840320
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H	-0.073516	-1.027115	4.090364
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H	1.446462	-1.943922	4.230631
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H	-1.806274	1.526464	-0.137938
C	-3.288148	0.351662	-1.105194

C	-4.279755	1.290213	-1.410164
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C	-5.615007	0.916958	-1.511990
H	-3.991775	2.329343	-1.570178
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C	-5.986482	-0.412883	-1.311883
H	-6.370432	1.662563	-1.749131
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Fe2-cpt-2

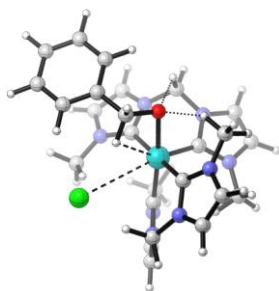


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C	-0.702728	-4.187251	-0.478734
H	-0.594650	-5.171282	-0.050378
C	-0.488277	-2.929425	1.714596
H	-1.380713	-2.483656	2.182329
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C	0.661900	-0.789745	1.423720
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H	1.988190	-3.321824	3.069657
C	2.612725	-1.269784	2.490265
H	3.614918	-1.082165	2.842783
C	2.396867	0.992752	1.435724
H	1.891109	1.316791	0.522373
H	3.469997	0.934423	1.241575
H	2.211367	1.703016	2.249779
C	-1.074337	-1.566651	-2.923182

H	-0.550702	-2.043168	-3.754548
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H	-2.125107	-1.425192	-3.200682
C	-2.191649	0.699717	-0.958043
C	-4.041209	1.211847	-2.173975
H	-5.032751	1.059301	-2.570366
C	-3.171135	2.241810	-2.327768
H	-3.247229	3.161188	-2.886702
C	-0.869425	2.712998	-1.356789
H	0.000835	2.165026	-1.740468
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C	-0.667255	1.830498	0.910618
C	-0.660479	4.108790	0.756385
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H	-0.546316	4.402452	2.952583
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H	-3.692036	-1.196947	0.088672
H	-3.766158	-1.767966	-1.618092
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H	0.495000	1.424623	3.653878
H	-1.112829	0.717748	3.252621
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Fe2-ncp-TSIM1

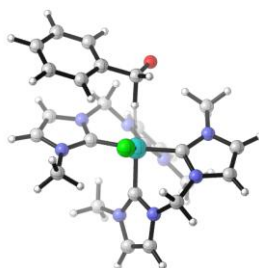


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C	-2.363002	-1.193506	3.313057
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C	-2.894768	-2.051511	2.410461
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C	-2.563532	-2.468618	-0.034478
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C	-3.505985	-0.592036	-2.948021
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C	-1.820531	1.254736	-3.120074
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H	0.240247	0.347444	3.637244
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O	0.708699	0.601454	-1.781299
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C	4.936622	0.613226	-1.344578
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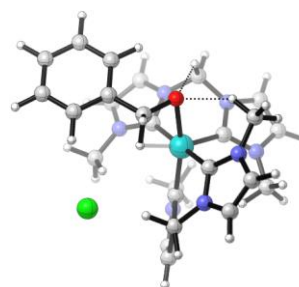
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C	0.086800	-1.391947	3.563826
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H	-2.364594	-0.849056	2.847498
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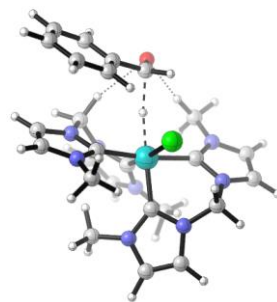
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C	-5.341065	-1.010776	-0.177896
H	-3.951759	-2.604606	0.334112
C	-4.464680	0.646069	-1.687734
H	-2.422687	0.353020	-2.329400
C	-5.516321	0.161500	-0.909283
H	-6.161351	-1.408050	0.417200
H	-4.594597	1.559005	-2.267224
H	-6.467443	0.688747	-0.882561

Fe2-ncp-IM1-i



O 1			
Fe	-0.397632	0.141827	-0.237516
N	-1.689143	-2.112346	1.134983
N	-1.099648	-0.671015	2.604514
N	-2.372373	-1.886149	-1.123245
N	-2.526033	-0.168637	-2.390402
N	-0.797841	2.962195	0.076994
N	-2.684274	1.994149	0.415802
N	1.390318	2.270540	0.680294
N	2.122243	0.454777	1.541604
C	-1.061446	-0.896524	1.247516
C	-1.663223	-1.736383	3.289445
H	-1.749596	-1.746495	4.364288
C	-2.028984	-2.648640	2.358648
H	-2.470332	-3.627397	2.456559
C	-1.831282	-2.797309	-0.132222
H	-0.830681	-3.182397	-0.418276
H	-2.523468	-3.632029	-0.003806
C	-1.817286	-0.656368	-1.329482
C	-3.389380	-2.157868	-2.017165
H	-3.922595	-3.095484	-2.023187
C	-3.488773	-1.065995	-2.818379
H	-4.138190	-0.858821	-3.654446
C	-2.316492	1.151752	-2.952408
H	-1.267748	1.411063	-2.790597
H	-2.973842	1.890340	-2.476955
H	-2.531615	1.127078	-4.022568

C	-0.655639	0.536552	3.264125
H	-1.298940	0.734354	4.124933
H	-0.719913	1.373470	2.567471
H	0.379672	0.453037	3.611539
C	-1.374408	1.710460	0.101177
C	-2.896951	3.357385	0.559182
H	-3.866963	3.763742	0.798742
C	-1.705569	3.968432	0.355536
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C	0.615411	3.126188	-0.190816
H	0.819257	2.835177	-1.226995
H	0.891764	4.168185	-0.014092
C	1.118822	0.932350	0.756193
C	2.536120	2.613934	1.375083
H	2.924294	3.620045	1.403028
C	2.994255	1.459497	1.920286
H	3.866435	1.260363	2.522745
C	-3.734714	1.006352	0.533957
H	-3.297212	0.053318	0.832356
H	-4.258746	0.863811	-0.418192
H	-4.454704	1.328681	1.289405
C	2.280154	-0.938722	1.926353
H	3.325808	-1.228771	1.808007
H	1.677605	-1.596743	1.287084
H	1.981876	-1.084344	2.971052
C	1.160456	-0.466098	-1.781453
H	0.928637	-1.187837	-2.592407
C	2.655742	-0.388630	-1.550556
C	3.385360	-1.521320	-1.175370
C	3.314374	0.832905	-1.698416
C	4.752562	-1.417237	-0.933542
H	2.862832	-2.466852	-1.015798
C	4.683049	0.932489	-1.460821
H	2.728340	1.699363	-1.995957
C	5.406126	-0.192801	-1.071719
H	5.308734	-2.299777	-0.626197
H	5.186423	1.890040	-1.578501
H	6.474389	-0.117667	-0.882316
H	0.758303	-1.100385	-0.869052
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Cl	1.158232	-3.773884	0.333958

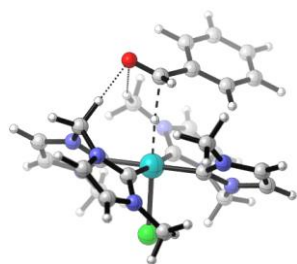


Fe2-ncp-TS1-o

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	N	2.899572	-0.827466	-1.670331
	N	2.072763	-2.535205	-0.683412
	N	-0.360773	-0.737793	2.415890
	N	1.781701	-0.749074	2.327939
	N	-1.940676	0.647964	1.326467
	N	-1.649762	2.282263	-0.019714
	C	1.808218	1.385729	-0.180665
	C	3.281803	3.038608	0.428222
	H	3.652093	3.858968	1.023030
	C	3.784566	2.450234	-0.682718
	H	4.676690	2.656652	-1.253489
	C	3.055724	0.532088	-2.138554
	H	2.293199	0.734305	-2.898405
	H	4.064020	0.652136	-2.542224
	C	1.813123	-1.213242	-0.922229
	C	3.793352	-1.861695	-1.882434
	H	4.685151	-1.748177	-2.478915
	C	3.265101	-2.941711	-1.256980
	H	3.614868	-3.959854	-1.187883
	C	1.253687	-3.397899	0.150316
	H	0.187222	-3.211427	-0.015317
	H	1.490266	-3.248143	1.210392
	H	1.467176	-4.436487	-0.109939
	C	1.296230	2.701537	1.887812
	H	1.899340	2.618391	2.798230
	H	0.470530	1.992888	1.940762
	H	0.893019	3.717504	1.822805
	C	0.673245	-0.533406	1.526633
	C	1.426803	-1.077100	3.628822
	H	2.164162	-1.291677	4.386438
	C	0.074691	-1.063177	3.685576
	H	-0.605253	-1.266437	4.497979
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	H	-1.967834	-1.454195	1.311010
	H	-2.387401	-0.675225	2.861100

C	-1.099242	1.079814	0.328694
C	-2.977495	1.528267	1.566074
H	-3.758904	1.325614	2.281506
C	-2.794889	2.560464	0.708251
H	-3.380557	3.450289	0.538567
C	3.161086	-0.687712	1.902593
H	3.207029	-0.273745	0.897752
H	3.612886	-1.686237	1.890313
H	3.737511	-0.047781	2.578788
C	-1.121987	3.164804	-1.038245
H	-1.689098	3.066871	-1.967788
H	-0.094215	2.872807	-1.252343
H	-1.167481	4.199122	-0.682649
Cl	-0.037652	0.557827	-2.636998
O	-1.816088	-3.158338	-0.256331
C	-1.870374	-2.134499	-0.983333
H	-1.351593	-2.091662	-1.965968
H	-0.779113	-1.134603	-0.462347
C	-3.105545	-1.271029	-0.926374
C	-4.142703	-1.655701	-0.070280
C	-3.271204	-0.138846	-1.730031
C	-5.319497	-0.915676	-0.001849
H	-3.998863	-2.559224	0.518452
C	-4.446127	0.603670	-1.657066
H	-2.456688	0.160410	-2.387643
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H	-6.124698	-1.231483	0.658339
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H	-6.392984	0.799332	-0.747952

Fe2-cp-TS1-o

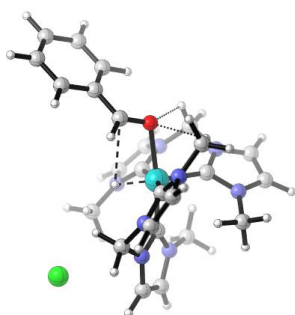


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N	1.826191	-1.651605	0.928515
N	-2.917087	-0.110782	-1.503528
N	-3.163602	1.697640	-0.389006
N	-2.128473	-2.207961	-0.736560

N	-1.482152	-2.737233	1.231001
C	0.155250	1.877779	0.346225
C	0.939583	3.991316	-0.091318
H	1.045085	4.906800	-0.652106
C	1.498379	3.595045	1.077002
H	2.175168	4.100482	1.748395
C	1.370767	1.497240	2.457844
H	0.491014	1.380786	3.101097
H	2.192386	1.976480	2.995565
C	1.048371	-0.537940	1.126086
C	2.991743	-0.429404	2.341998
H	3.712446	0.009601	3.013912
C	2.998666	-1.601003	1.662742
H	3.739186	-2.383765	1.611657
C	1.499121	-2.758449	0.049657
H	0.925753	-2.402583	-0.809083
H	2.428053	-3.201676	-0.313713
H	0.923538	-3.527810	0.575039
C	-0.526912	2.960243	-1.809057
H	0.185962	3.229026	-2.594789
H	-0.914248	1.961269	-2.005895
H	-1.355062	3.677574	-1.824428
C	-2.298408	0.642006	-0.534051
C	-4.255134	1.596113	-1.235800
H	-5.038497	2.337715	-1.252449
C	-4.107302	0.444780	-1.934489
H	-4.728104	-0.017871	-2.685767
C	-2.377555	-1.393410	-1.907497
H	-1.441557	-1.271734	-2.468431
H	-3.112955	-1.899902	-2.537155
C	-1.409258	-1.714132	0.321856
C	-2.619411	-3.478370	-0.503027
H	-3.208385	-4.018160	-1.227783
C	-2.199721	-3.815695	0.740270
H	-2.357646	-4.710742	1.321420
C	-2.984357	2.798584	0.535145
H	-2.237291	2.508727	1.274746
H	-2.675237	3.708303	0.006155
H	-3.925223	2.995932	1.054019
C	-0.866897	-2.732121	2.542720
H	0.051220	-3.332715	2.547242
H	-0.651369	-1.699353	2.818739
H	-1.564658	-3.149275	3.272269
Cl	-1.677434	0.504818	2.578945
O	0.499627	-1.500243	-2.981176
C	0.880158	-0.422021	-2.466502
H	0.456464	0.547578	-2.821538

H	0.105434	-0.210313	-1.130130
C	2.300783	-0.276732	-1.992131
C	2.776526	0.903204	-1.416150
C	3.187534	-1.336986	-2.188713
C	4.097544	1.005422	-0.995892
H	2.098646	1.742281	-1.288476
C	4.514104	-1.236086	-1.779149
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H	4.447178	1.926216	-0.533303
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H	6.004824	0.009989	-0.844794

Fe2-ncp-TS1-i

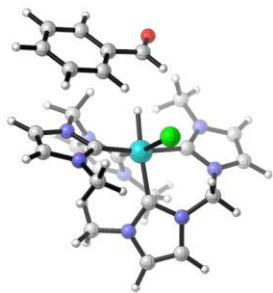


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N	0.547482	-1.029718	3.147488
N	0.121320	3.053711	0.562322
N	1.930707	2.376120	1.488764
N	-0.976594	2.205161	-1.381475
N	-0.428727	0.541027	-2.622811
C	1.868039	-0.291308	-0.532495
C	3.784554	-0.393557	-1.772907
H	4.526191	-0.033616	-2.467594
C	3.610816	-1.608632	-1.206066
H	4.120241	-2.547620	-1.346399
C	1.851435	-2.613658	0.260611
H	0.975402	-2.938136	-0.314946
H	2.550529	-3.448342	0.314119
C	0.761154	-1.034238	1.790786
C	1.695901	-2.868898	2.777513
H	2.237396	-3.801226	2.812925
C	1.102453	-2.143741	3.759567
H	1.028265	-2.317102	4.821702
C	-0.126984	0.041074	3.843477

H	-0.279859	0.853640	3.130329
H	0.481112	0.392293	4.682903
H	-1.101106	-0.281805	4.224756
C	2.553115	1.759042	-1.817282
H	3.450387	2.351789	-1.607407
H	1.703532	2.212931	-1.311804
H	2.367556	1.778467	-2.897561
C	0.776357	1.887857	0.917281
C	1.990988	3.760474	1.458771
H	2.824010	4.311016	1.867657
C	0.851535	4.191483	0.867058
H	0.490008	5.188122	0.665750
C	-1.113729	3.021463	-0.194081
H	-1.908003	2.614654	0.436818
H	-1.368910	4.040759	-0.493075
C	-0.448131	0.935842	-1.315070
C	-1.261286	2.587057	-2.683493
H	-1.701832	3.540268	-2.931856
C	-0.917112	1.528600	-3.458973
H	-0.986508	1.386606	-4.526159
C	3.007520	1.537851	1.967854
H	2.663678	0.503122	1.948823
H	3.286165	1.818217	2.988019
H	3.887505	1.623464	1.321426
C	0.100405	-0.734354	-3.096829
H	-0.460479	-1.054439	-3.975693
H	0.018858	-1.492281	-2.317179
H	1.159724	-0.658854	-3.358247
C	-2.383801	-0.634305	1.016057
H	-0.317379	-1.236713	-0.293674
O	-1.765245	0.441036	1.103195
Cl	1.742663	-3.718488	-2.652867
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C	-3.755355	-0.732862	0.547487
C	-4.394647	-1.981162	0.547008
C	-4.440925	0.396957	0.072725
C	-5.701737	-2.097041	0.093909
H	-3.849171	-2.854659	0.897621
C	-5.745936	0.278564	-0.377297
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C	-6.378155	-0.967504	-0.365540
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Fe2-ncp-IM2-o

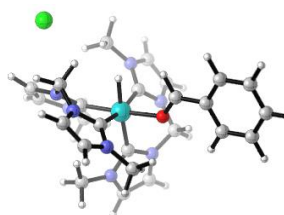


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N	1.855684	-1.171505	1.062508
N	1.416660	-2.333528	-0.677180
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C	-3.586079	-2.835228	-0.358706
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C	-4.035912	-1.914501	-1.244051
H	-4.949467	-1.867373	-1.816605
C	-3.112437	0.252632	-2.136544
H	-2.343678	0.213058	-2.917330
H	-4.113100	0.332791	-2.568517
C	-1.761953	1.481102	-0.488290
C	-3.601242	2.582885	-1.306442
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C	-2.963711	3.422141	-0.453623
H	-3.188334	4.435886	-0.161120
C	-0.898261	3.321110	0.952678
H	0.063346	3.487776	0.459179
H	-0.734274	2.648998	1.798300
H	-1.294489	4.270868	1.318098
C	-1.555295	-3.109924	1.054617
H	-2.134534	-3.245231	1.974460
H	-0.670710	-2.512691	1.275766
H	-1.243194	-4.093425	0.686980
C	-0.677239	0.041536	1.661268
C	-1.351177	0.058531	3.862170
H	-2.057201	0.107799	4.676485
C	-0.002402	-0.054310	3.866047
H	0.702418	-0.120502	4.680223
C	1.738401	-0.116064	2.036671
H	1.969185	0.839820	1.545085
H	2.430085	-0.301195	2.862256

C	0.982584	-1.220432	-0.001235
C	2.770211	-2.207213	1.056939
H	3.545432	-2.306112	1.800790
C	2.495153	-2.936617	-0.051483
H	2.978280	-3.812081	-0.457194
C	-3.136049	0.246011	2.144885
H	-3.204683	0.157825	1.062110
H	-3.533049	1.223392	2.442264
H	-3.744407	-0.538417	2.608017
C	0.819943	-2.834192	-1.896425
H	1.400690	-2.525133	-2.769983
H	-0.174231	-2.398055	-1.997130
H	0.765333	-3.926819	-1.854609
Cl	0.040523	0.237198	-2.652288
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C	2.329215	2.524670	-0.774740
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H	0.588960	1.150764	0.024503
C	3.388302	1.495317	-0.688117
C	4.414018	1.625670	0.255273
C	3.370978	0.397945	-1.556709
C	5.418010	0.668401	0.329960
H	4.398056	2.493197	0.911218
C	4.382985	-0.553710	-1.483926
H	2.538584	0.296856	-2.254801
C	5.404664	-0.420387	-0.544460
H	6.219722	0.770622	1.057446
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H	6.193777	-1.167107	-0.491012

Fe2-ncp-IM2-i



0 1

Fe	-0.172477	0.007586	0.065463
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N	0.563171	-2.630317	1.151504
N	-0.586075	-1.621799	2.651657
N	0.280107	-2.598347	-1.218456
N	-1.134915	-1.492731	-2.396188

C	-2.093208	0.125755	0.181190
C	-4.356259	-0.184123	0.212487
H	-5.270135	-0.756007	0.209270
C	-4.137358	1.146040	0.102733
H	-4.799861	1.973853	-0.090870
C	-2.079454	2.562665	-0.069910
H	-1.666843	2.584266	-1.085319
H	-2.787473	3.385348	0.026521
C	-0.120501	1.665626	1.101715
C	-0.743512	3.776271	1.707650
H	-1.348130	4.669224	1.687872
C	0.372483	3.468529	2.414558
H	0.933210	4.038924	3.138221
C	1.845573	1.451563	2.607223
H	1.714678	0.394977	2.363247
H	1.868562	1.582378	3.693066
H	2.800199	1.789728	2.190684
C	-2.961111	-2.230798	0.329349
H	-3.386024	-2.625154	1.259682
H	-1.906095	-2.492741	0.285655
H	-3.473924	-2.703631	-0.515456
C	-0.026345	-1.408023	1.414051
C	-0.373965	-2.912111	3.111729
H	-0.740409	-3.252263	4.067839
C	0.344943	-3.555259	2.160727
H	0.733940	-4.561211	2.125235
C	1.181061	-2.907781	-0.130949
H	2.091357	-2.308970	-0.227529
H	1.441073	-3.967738	-0.174546
C	-0.347763	-1.376066	-1.287306
C	-0.115443	-3.448073	-2.240486
H	0.287969	-4.440711	-2.366919
C	-1.004930	-2.739844	-2.980429
H	-1.545260	-3.006683	-3.875145
C	-1.369579	-0.631847	3.357640
H	-1.375133	0.279151	2.757420
H	-0.935755	-0.424263	4.340716
H	-2.400908	-0.974271	3.489359
C	-2.042748	-0.456704	-2.881484
H	-2.093159	-0.499191	-3.969960
H	-1.688067	0.527076	-2.573496
H	-3.050162	-0.578238	-2.473713
C	2.484999	0.699550	-0.912293
H	-0.233267	1.012081	-1.134271
O	1.824091	0.015678	-0.104514
Cl	-3.752900	2.502274	-2.696093
H	1.946891	1.339326	-1.632389

C	3.931743	0.691663	-0.940410
C	4.607453	1.463017	-1.900887
C	4.679533	-0.071628	-0.023908
C	5.994540	1.468316	-1.948310
H	4.027296	2.053446	-2.606809
C	6.063985	-0.061662	-0.075195
H	4.146498	-0.657284	0.721452
C	6.725952	0.706412	-1.037175
H	6.509838	2.065854	-2.694590
H	6.638172	-0.650737	0.634705
H	7.811532	0.711218	-1.073934

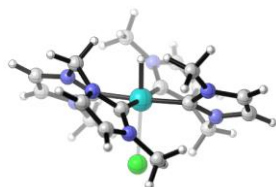
Fe2-ncp-3



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N	2.884535	0.758636	-0.703055
N	2.859393	-1.374914	-0.575807
N	-1.553120	-1.950968	0.952548
N	0.137190	-1.382518	2.137192
N	-2.812859	-0.665212	-0.595085
N	-2.547599	1.344789	-1.276586
C	0.321472	1.502190	0.358899
C	0.257748	3.290139	1.810616
H	-0.142997	3.903197	2.602993
C	1.370979	3.438503	1.055217
H	2.130805	4.204679	1.054434
C	2.375931	2.099250	-0.834938
H	1.881543	2.181056	-1.814100
H	3.196918	2.815107	-0.744470
C	2.007675	-0.301425	-0.645168
C	4.210347	0.363716	-0.690339
H	5.030880	1.062090	-0.744436
C	4.188857	-0.989209	-0.614569
H	4.994591	-1.706188	-0.586347
C	2.435650	-2.754414	-0.457748
H	1.408512	-2.768753	-0.093583
H	3.102291	-3.277586	0.235809
H	2.438154	-3.248564	-1.431240
C	-1.588828	1.636995	1.988488

H	-1.477414	1.540922	3.074120
H	-1.817421	0.659121	1.567363
H	-2.426072	2.313580	1.780325
C	-0.390267	-1.212403	0.871374
C	-0.667127	-2.174358	2.942775
H	-0.401617	-2.422441	3.958809
C	-1.740223	-2.527858	2.195548
H	-2.593139	-3.147103	2.427428
C	-2.482305	-2.004771	-0.158050
H	-2.001033	-2.530792	-0.992463
H	-3.395097	-2.509184	0.168232
C	-1.824394	0.243080	-0.891791
C	-4.083526	-0.154705	-0.789473
H	-4.977230	-0.739720	-0.636846
C	-3.913215	1.118918	-1.220895
H	-4.633148	1.869503	-1.507621
C	1.361298	-0.769768	2.597474
H	1.737865	-0.126474	1.801659
H	2.115861	-1.527478	2.835124
H	1.177441	-0.164614	3.491985
C	-1.947490	2.600563	-1.665077
H	-2.554877	3.074366	-2.439742
H	-0.947140	2.378744	-2.046525
H	-1.859649	3.283900	-0.811383
H	0.332359	0.824484	-1.926930
Cl	-0.098031	-1.957622	-2.253287

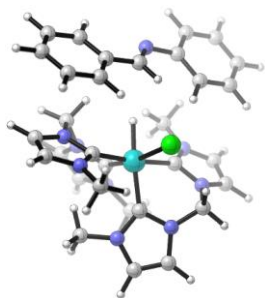
Fe2-cp-3



O 1			
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N	2.656416	1.184106	0.271882
N	1.519718	2.468122	-1.009270
N	-2.637237	-1.183934	-0.628491
N	-1.583913	-2.539577	0.646690
N	-2.637101	1.184269	-0.628478
N	-1.583620	2.539774	0.646721
C	1.397733	-1.312612	-0.271672
C	2.787789	-3.019501	-0.913092
H	3.059237	-3.931852	-1.421072
C	3.512147	-2.201067	-0.112420

H	4.536056	-2.259872	0.222810
C	3.010958	-0.000190	1.027944
H	2.448586	-0.000143	1.968895
H	4.088983	-0.000267	1.205593
C	1.397921	1.312449	-0.271693
C	3.512472	2.200587	-0.112463
H	4.536393	2.259238	0.222757
C	2.788226	3.019136	-0.913117
H	3.059806	3.931447	-1.421098
C	0.478017	2.991152	-1.863434
H	-0.172227	2.158945	-2.143416
H	0.925642	3.429496	-2.758879
H	-0.120474	3.757921	-1.357319
C	0.477537	-2.991242	-1.863311
H	0.925063	-3.429646	-2.758776
H	-0.172617	-2.158955	-2.143263
H	-0.121025	-3.757933	-1.357162
C	-1.429738	-1.328632	0.017925
C	-2.816793	-3.113179	0.380300
H	-3.110411	-4.063257	0.799110
C	-3.490932	-2.253318	-0.421202
H	-4.482905	-2.301864	-0.842886
C	-2.905505	0.000188	-1.406226
H	-2.242302	0.000157	-2.282316
H	-3.952902	0.000253	-1.718702
C	-1.429581	1.328826	0.017930
C	-3.490658	2.253767	-0.421207
H	-4.482613	2.302448	-0.842917
C	-2.816458	3.113494	0.380389
H	-3.109988	4.063575	0.799254
C	-0.574234	-3.160130	1.479347
H	0.081805	-2.374246	1.860763
H	0.005964	-3.899407	0.912782
H	-1.057134	-3.661171	2.321373
C	-0.573874	3.160177	1.479406
H	0.006445	3.899382	0.912867
H	0.082047	2.374193	1.860821
H	-1.056724	3.661274	2.321428
H	-0.196149	0.000026	-1.622257
Cl	0.151539	0.000029	2.466390

Fe2-ncp-IM3-o

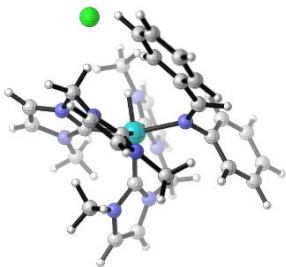


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Fe	0.583420	0.470185	-0.173328
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N	2.919466	-1.109262	-1.045901
N	2.011975	-2.106420	0.616438
N	-0.300130	0.919494	2.533500
N	1.836366	0.702126	2.563038
N	-1.674175	1.969943	0.933582
N	-1.144348	2.917186	-0.907773
C	2.079597	1.625648	-0.687545
C	3.757888	3.194759	-0.784036
H	4.241926	4.135764	-0.572911
C	4.154845	2.144731	-1.542035
H	5.048401	1.989630	-2.126955
C	3.149509	-0.109815	-2.067559
H	2.347652	-0.178791	-2.811601
H	4.128349	-0.282495	-2.520980
C	1.840783	-1.015034	-0.197351
C	3.721431	-2.202984	-0.769166
H	4.596138	-2.447897	-1.351589
C	3.138834	-2.835561	0.279131
H	3.401915	-3.749864	0.788451
C	1.108125	-2.479489	1.683970
H	0.167113	-1.949388	1.519892
H	1.519539	-2.204704	2.662848
H	0.926064	-3.557743	1.649842
C	1.788940	3.720378	0.647026
H	2.432047	4.002570	1.487223
H	0.931735	3.163850	1.026265
H	1.434372	4.631892	0.153748
C	0.766618	0.693954	1.681059
C	1.429359	0.910971	3.873871
H	2.129838	0.937121	4.694083
C	0.083613	1.055772	3.854224
H	-0.623590	1.229535	4.650270
C	-1.639567	1.004688	2.003129
H	-1.920857	0.024454	1.592195
H	-2.330609	1.306292	2.793934

C	-0.813198	1.834212	-0.131609
C	-2.471031	3.094700	0.842906
H	-3.225173	3.336769	1.575558
C	-2.140406	3.687659	-0.329835
H	-2.540521	4.565469	-0.813441
C	3.222793	0.521919	2.201792
H	3.304720	0.507367	1.116198
H	3.614291	-0.423437	2.594975
H	3.829452	1.344766	2.595015
C	-0.526185	3.238746	-2.175472
H	-1.244743	3.119191	-2.992139
H	0.289971	2.536437	-2.345187
H	-0.160182	4.271437	-2.165778
Cl	-0.014228	-0.020849	-2.571320
C	-2.647829	-1.616787	-0.753517
H	-0.546194	-0.562334	0.168931
N	-2.596621	-2.634104	0.036086
H	-1.979686	-1.479920	-1.614998
C	-3.621104	-0.547117	-0.574863
C	-4.578996	-0.569348	0.450055
C	-3.594313	0.534974	-1.467581
C	-5.498090	0.464519	0.569503
H	-4.583315	-1.417731	1.129689
C	-4.523398	1.562513	-1.349513
H	-2.818148	0.554704	-2.233298
C	-5.478176	1.529452	-0.334432
H	-6.245301	0.438974	1.359235
H	-4.497063	2.397871	-2.045523
H	-6.206003	2.332349	-0.244453
C	-1.593769	-3.590188	-0.173302
C	-0.460770	-3.400769	-0.988651
C	-1.719855	-4.797308	0.532379
C	0.490154	-4.407966	-1.099829
H	-0.298501	-2.453120	-1.501561
C	-0.760843	-5.796831	0.419195
H	-2.592260	-4.923018	1.168289
C	0.352179	-5.607333	-0.400235
H	1.364601	-4.240255	-1.725551
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H	1.105378	-6.386210	-0.491052

Fe2-ncp-IM3-i

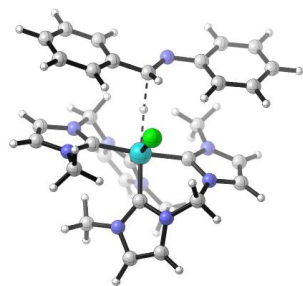


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N	-2.420678	-0.786562	1.270845
N	-1.683107	1.000739	2.179598
N	3.024840	-0.041834	1.306029
N	1.652191	-0.676252	2.818046
N	2.995217	-0.381965	-1.061469
N	1.553204	-1.213891	-2.410254
C	-0.072220	-2.138836	0.322592
C	-0.001342	-4.428879	0.306704
H	0.468186	-5.398676	0.264506
C	-1.304115	-4.070258	0.373636
H	-2.208067	-4.657592	0.375604
C	-2.529762	-1.894990	0.350940
H	-2.688064	-1.569447	-0.698614
H	-3.375433	-2.519610	0.648393
C	-1.325112	0.032007	1.271265
C	-3.426526	-0.332630	2.099478
H	-4.374968	-0.838761	2.187347
C	-2.962115	0.802332	2.675659
H	-3.421647	1.482768	3.375147
C	-0.827970	2.085389	2.587089
H	0.194107	1.831683	2.292236
H	-0.878640	2.220399	3.672285
H	-1.117611	3.026355	2.102581
C	2.178755	-3.249625	0.211024
H	2.585284	-2.418378	0.785605
H	2.521565	-3.157869	-0.826054
H	2.560041	-4.185882	0.624461
C	1.662933	-0.188017	1.520095
C	2.923745	-0.830955	3.343493
H	3.091758	-1.199981	4.343312
C	3.795605	-0.437568	2.387675
H	4.873341	-0.387172	2.383427
C	3.584828	0.350665	0.035404
H	3.460396	1.426005	-0.117750
H	4.656426	0.133165	0.054413
C	1.637349	-0.591920	-1.189911

C	3.710241	-0.836273	-2.155063
H	4.781744	-0.736108	-2.233888
C	2.791773	-1.364378	-3.002249
H	2.909656	-1.834249	-3.966192
C	0.464861	-1.106180	3.526547
H	-0.166001	-1.705232	2.865795
H	-0.122608	-0.256770	3.885218
H	0.767897	-1.709397	4.384233
C	0.314601	-1.691124	-3.015755
H	0.551870	-2.137113	-3.982607
H	-0.405794	-0.882901	-3.147168
H	-0.186079	-2.428171	-2.385203
C	-1.020052	2.556891	-0.596566
N	0.017922	1.783608	-0.444596
C	-2.437194	2.218523	-0.617346
C	-3.337684	3.161733	-0.088330
C	-2.949841	1.073239	-1.244851
C	-4.706579	2.929859	-0.122796
H	-2.949931	4.078124	0.356801
C	-4.321695	0.856298	-1.301889
H	-2.292126	0.347429	-1.716950
C	-5.201247	1.772933	-0.727110
H	-5.389497	3.659091	0.305523
H	-4.662254	-0.041752	-1.816741
H	-6.274055	1.601189	-0.768651
C	1.239869	2.487531	-0.670052
C	1.859839	2.387968	-1.920117
C	1.798032	3.308115	0.314122
C	3.051127	3.063920	-2.160794
H	1.400801	1.763316	-2.682033
C	2.987892	3.988255	0.063904
H	1.294665	3.407156	1.271711
C	3.625878	3.859839	-1.168637
H	3.528640	2.973738	-3.133017
H	3.414752	4.623358	0.835511
H	4.554577	4.388925	-1.361346
H	-0.742749	-0.517286	-0.998966
H	-0.818043	3.628878	-0.735572
Cl	-2.986261	-2.047429	-2.863169

Fe2-ncp-TS2-o

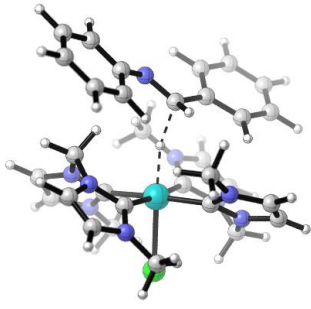


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N	-2.631966	-0.825539	0.719322
N	1.108713	-0.034018	2.498509
N	-0.013574	-1.860013	2.530466
N	2.611492	0.767925	0.867173
N	3.218144	-0.107993	-0.984823
C	0.635911	-2.470442	-0.638191
C	1.377019	-4.640864	-0.724503
H	2.043623	-5.463899	-0.519199
C	0.239392	-4.581477	-1.456349
H	-0.281710	-5.339319	-2.020518
C	-1.428460	-2.764827	-1.971778
H	-1.185075	-2.058286	-2.772016
H	-2.007350	-3.610545	-2.349682
C	-1.630180	-1.115708	-0.165756
C	-3.501545	-2.373266	-0.581351
H	-4.116977	-3.081707	-1.113517
C	-3.774022	-1.563649	0.471193
H	-4.684487	-1.412178	1.029872
C	-2.536026	0.168571	1.769071
H	-1.688162	0.821037	1.553452
H	-2.393790	-0.310080	2.745832
H	-3.443991	0.776992	1.782022
C	2.701893	-3.052459	0.655442
H	2.709644	-3.743466	1.504631
H	2.572691	-2.035687	1.024150
H	3.662114	-3.122742	0.133855
C	0.402829	-0.868733	1.657009
C	0.417954	-1.623686	3.828058
H	0.173526	-2.289032	4.641314
C	1.134112	-0.475601	3.807228
H	1.636647	0.064786	4.594026
C	1.752227	1.140781	1.964796
H	0.986296	1.835244	1.602668
H	2.346035	1.622813	2.744417
C	2.113166	0.040601	-0.189895

C	3.955772	1.053913	0.735385
H	4.497020	1.652766	1.450926
C	4.336326	0.504536	-0.442864
H	5.288395	0.510911	-0.950172
C	-0.809062	-3.019465	2.194763
H	-0.901415	-3.092279	1.113724
H	-1.813316	-2.945573	2.626773
H	-0.327640	-3.927559	2.572344
C	3.238229	-0.805482	-2.253599
H	3.203033	-0.095921	-3.084943
H	2.349978	-1.432490	-2.323144
H	4.149102	-1.408466	-2.323106
Cl	0.087902	-0.088994	-2.630343
C	-0.483195	2.498144	-0.553325
H	-0.161700	1.089988	-0.076992
N	-1.465108	3.019265	0.185100
H	-0.676196	2.095171	-1.556925
C	0.845404	3.163650	-0.480519
C	1.143874	4.107725	0.508316
C	1.810040	2.873461	-1.453915
C	2.388536	4.730474	0.537417
H	0.367489	4.348476	1.230562
C	3.048277	3.506652	-1.431666
H	1.565571	2.135901	-2.218221
C	3.345893	4.432867	-0.432648
H	2.607059	5.468371	1.306416
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H	4.312924	4.930147	-0.416948
C	-2.755150	2.644455	-0.126364
C	-3.126905	1.667934	-1.083966
C	-3.796699	3.257934	0.607117
C	-4.462664	1.331603	-1.271972
H	-2.363268	1.146582	-1.659419
C	-5.126017	2.915823	0.409045
H	-3.513303	4.008205	1.341615
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H	-4.715167	0.567838	-2.006216
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Fe2-cp-TS2-o

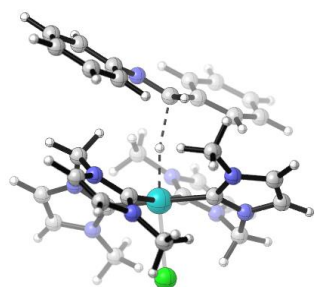


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N	-0.751208	-0.540791	-2.974718
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N	-0.156804	-1.652897	3.089162
N	2.589918	-1.334563	0.129935
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C	-3.539600	1.042373	1.897667
H	-3.899705	1.772228	2.605667
C	-4.198094	0.306176	0.970499
H	-5.245254	0.249833	0.717737
C	-3.437530	-1.319188	-0.804195
H	-3.242733	-2.349259	-0.483996
H	-4.463924	-1.204458	-1.161423
C	-1.174636	-0.852210	-1.700380
C	-2.925400	-0.765702	-3.192210
H	-3.953762	-0.839356	-3.510505
C	-1.795864	-0.483180	-3.883132
H	-1.641023	-0.247406	-4.924237
C	0.610337	-0.230722	-3.342018
H	1.229301	-0.335427	-2.451915
H	0.686386	0.795277	-3.717187
H	0.968745	-0.916133	-4.116958
C	-1.165149	1.370235	2.578119
H	-1.507040	2.362143	2.878747
H	-0.250399	1.477414	1.990066
H	-0.947780	0.778743	3.474350
C	0.369039	-1.178950	1.914480
C	0.782861	-1.665063	4.107280
H	0.543945	-2.011760	5.100476
C	1.945828	-1.207801	3.582129
H	2.922177	-1.069684	4.019166
C	2.572873	-0.424442	1.251296
H	2.214636	0.551148	0.920243
H	3.581246	-0.320598	1.658045

C	1.416314	-1.696879	-0.488685
C	3.690195	-2.005622	-0.365929
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C	3.218678	-2.823319	-1.337746
H	3.727620	-3.522316	-1.982813
C	-1.537991	-2.042040	3.294136
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H	-1.572827	-2.889436	3.982003
C	0.984670	-3.378742	-2.286038
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H	2.534108	1.036156	-1.764029
C	5.050421	3.070719	0.351852
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H	4.938820	0.758279	-2.128335
H	5.756729	3.638502	0.953389
H	6.585621	2.045137	-0.775217
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Fe2-cpt-TS2-o

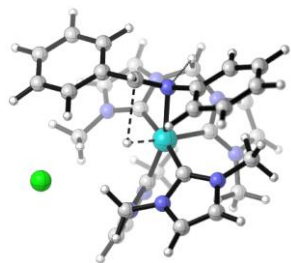


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N	-0.903714	-0.570253	-2.929377
N	1.677977	-0.901583	2.202632
N	-0.097555	-1.682162	3.102766
N	2.565394	-1.318448	0.061912
N	1.827667	-2.693580	-1.398207
C	-1.983852	-0.124584	0.836207
C	-3.440572	1.233672	1.917807
H	-3.736962	2.027999	2.584185
C	-4.168402	0.476160	1.059622
H	-5.224984	0.458193	0.845014
C	-3.525444	-1.270705	-0.665485
H	-3.299420	-2.290493	-0.325541
H	-4.568326	-1.172764	-0.973049
C	-1.303895	-0.893894	-1.657962
C	-3.094302	-0.683710	-3.075963
H	-4.135284	-0.692179	-3.358764
C	-1.974545	-0.439364	-3.798647
H	-1.843857	-0.182774	-4.837934
C	0.466152	-0.315236	-3.315550
H	1.062383	-0.244230	-2.405464
H	0.532009	0.629535	-3.862446
H	0.855396	-1.121606	-3.946185
C	-1.018471	1.451844	2.507724
H	-1.309912	2.453237	2.825806
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H	-0.770597	0.847124	3.386481
C	0.388903	-1.246241	1.901636
C	0.856803	-1.594428	4.102603
H	0.652934	-1.902336	5.116043
C	1.987133	-1.106449	3.532753
H	2.961173	-0.896097	3.944930
C	2.530462	-0.376931	1.160151
H	2.103521	0.565046	0.807543
H	3.541040	-0.208265	1.536405
C	1.403016	-1.754326	-0.507668

C	3.675592	-1.953745	-0.455196
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C	3.206591	-2.826358	-1.381952
H	3.722837	-3.522734	-2.023632
C	-1.463313	-2.115065	3.327512
H	-1.838990	-2.564954	2.404353
H	-2.095059	-1.269623	3.626167
H	-1.475518	-2.863852	4.121591
C	0.947263	-3.520044	-2.199416
H	1.360379	-3.624670	-3.206957
H	-0.037891	-3.054911	-2.228188
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C	3.273908	1.643209	-1.278505
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C	4.625639	1.366307	-1.448863
H	2.551057	1.147300	-1.921012
C	5.171185	2.843842	0.364004
H	3.494041	3.800610	1.325563
C	5.590550	1.955576	-0.632788
H	4.929166	0.671130	-2.230787
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H	0.711172	1.896601	-1.695814
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C	-0.820096	2.840705	-0.517375
C	-1.873798	2.413618	-1.341517
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C	-3.152009	2.939265	-1.207368
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C	-2.372943	4.363705	0.568502
H	-0.265952	4.188195	1.045542
C	-3.413170	3.918367	-0.247196
H	-3.948832	2.587138	-1.860812
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Fe2-ncp-TS2-i

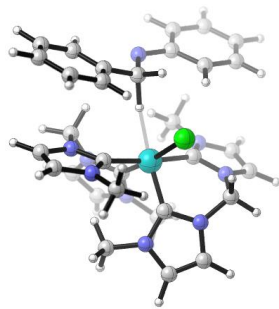


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N	-1.796313	-1.984456	2.164549
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N	2.699384	-0.011155	1.145974
C	0.658580	-1.978613	-0.311451
C	1.906098	-3.893975	-0.425577
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C	1.563441	-3.562383	-1.692657
H	1.822365	-4.005345	-2.640850
C	0.246104	-1.673222	-2.713540
H	0.851478	-0.764950	-2.864491
H	0.303903	-2.284545	-3.615968
C	-1.521450	-0.831599	-1.223559
C	-2.222298	-1.763279	-3.198723
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C	-3.332576	-1.443299	-2.489616
H	-4.380463	-1.542386	-2.726999
C	-3.800183	-0.545661	-0.225149
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H	-4.418253	-1.409014	0.045261
H	-4.453223	0.280239	-0.520359
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H	0.897523	-2.174000	2.283750
H	2.580450	-2.695369	2.085435
H	1.293154	-3.911853	2.261527
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C	-1.484448	-0.885267	4.047890
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H	-0.536683	1.775813	2.428238
H	-0.020724	1.306551	4.080851
C	1.344919	0.148186	1.258904

C	2.420281	0.808887	3.178799
H	2.508826	1.228239	4.169111
C	3.357324	0.381625	2.296341
H	4.433176	0.348984	2.372801
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C	1.972142	3.173209	0.662547
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C	3.343081	3.324150	0.835690
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H	5.289959	3.097331	-0.057685
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Fe2-ncp-IM4-o

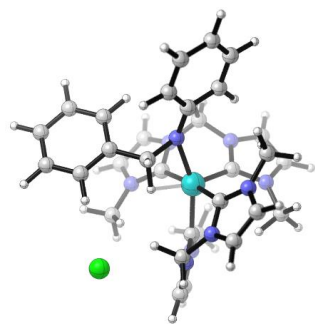


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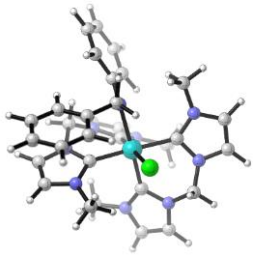


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C	3.501579	-2.748933	0.554425
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C	3.386491	-2.676183	-0.792499
H	4.065068	-2.946029	-1.584939
C	1.678294	-1.717303	-2.352984
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C	-0.641445	-1.591511	-1.505101
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Fe2-ncp-4

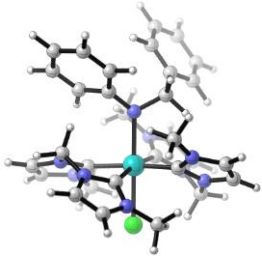


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17. References

1. M. Vellakkaran, K. Singh and D. Banerjee, An Efficient and Selective Nickel-Catalyzed Direct N-Alkylation of Anilines with Alcohols, *ACS Catalysis*, 2017, **7**, 8152-8158.
2. M. Huang, Y. Li, Y. Li, J. Liu, S. Shu, Y. Liu and Z. Ke, Room temperature N-heterocyclic carbene manganese catalyzed selective N-alkylation of anilines with alcohols, *Chemical Communications*, 2019, **55**, 6213-6216.
3. T. Scherg, S. K. Schneider, G. D. Frey, J. Schwarz, E. Herdtweck and W. A. Herrmann, Bridged Imidazolium Salts Used as Precursors for Chelating Carbene Complexes of Palladium in the Mizoroki-Heck Reaction, *Synlett*, 2006, **2006**, 2894-2907.
4. D. Brenna, M. Villa, T. N. Gieshoff, F. Fischer, M. Hapke and A. Jacobi von Wangelin, Iron-Catalyzed Cyclotrimerization of Terminal Alkynes by Dual Catalyst Activation in the Absence of Reductants, *Angew. Chem., Int. Ed.*, 2017, **56**, 8451-8454.
5. S. Meyer, C. M. Orben, S. Demeshko, S. Dechert and F. Meyer, Synthesis and Characterization of Di- and Tetracarbene Iron(II) Complexes with Chelating N-Heterocyclic Carbene Ligands and Their Application in Aryl Grignard-Alkyl Halide Cross-Coupling, *Organometallics*, 2011, **30**, 6692-6702.
6. A. Singh, A. Maji, M. Joshi, A. R. Choudhury and K. Ghosh, Designed pincer ligand supported Co(ii)-based catalysts for dehydrogenative activation of alcohols: Studies on N-alkylation of amines, α -alkylation of ketones and synthesis of quinolines, *Dalton Trans.*, 2021, **50**, 8567-8587.
7. H. S. Kunchur and M. S. Balakrishna, Platinum Assisted Tandem P-C Bond Cleavage and P-N Bond Formation in Amide Functionalized Bisphosphine *o*-Ph₂PC₆H₄C(O)N(H)C₆H₄PPh₂-*o*: Synthesis, Mechanistic, and Catalytic Studies, *Inorg. Chem.*, 2022, **61**, 857-868.
8. L. Homberg, A. Roller and K. C. Hultsch, A Highly Active PN₃ Manganese Pincer Complex Performing N-Alkylation of Amines under Mild Conditions, *Organic Letters*, 2019, **21**, 3142-3147.
9. D. Wu, Q. Bu, C. Guo, B. Dai and N. Liu, Cooperative catalysis of molybdenum with organocatalysts for distribution of products between amines and imines, *Molecular Catalysis*, 2021, **503**, 111415.
10. A. Singh, S. Gupta and J. M. Khurana, Zinc Chloride Mediated Nucleophilic Substitution: Amination and Thioetherification of Alcohols at Room Temperature, *Org. Prep. Proced. Int.*, 2020, **52**, 110-119.
11. J.-J. Ge, C.-Z. Yao, M.-M. Wang, H.-X. Zheng, Y.-B. Kang and Y. Li, Transition-Metal-Free Deacylative Cleavage of Unstrained C(sp³)-C(sp²) Bonds: Cyanide-Free Access to Aryl and Aliphatic Nitriles from Ketones and Aldehydes, *Org. Lett.*, 2016, **18**, 228-231.