

Supporting Information

NHC-catalyzed Silylative Dehydration of Primary Amides to Nitriles at Room Temperature

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1) General Information

1.1) General reagent information

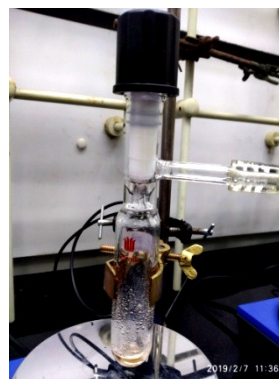
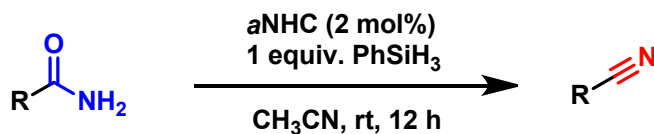
Unless stated otherwise, substrates were purchased from commercial vendors and used as supplied. PhSiH_3 was obtained from TCI chemicals and stored under inert atmosphere in the glovebox. Abnormal NHC (*a*NHC) was synthesized and stored under inert atmosphere at -25°C in the MBraun glovebox maintained below 0.1 ppm of O_2 and H_2O level. All other reagents were purchased from Sigma-Aldrich (Merck), Spectrochem, Alfa Aesar, TCI-India, Combi-Blocks, or Matrix Scientific and were used as received. THF, toluene, pentane, hexane and benzene were dried over a sodium/benzophenone mixture prior to use. Dry CH_3CN and DMSO were collected directly from Solvent Purification System (SPS). CDCl_3 was dried over CaH_2 and distilled before use. Analytical thin layer chromatography (TLC) was performed on a Merck 60 F254 silica gel plate (0.25 mm thickness). Column chromatography was performed on Merck 60 silica gel (100-200 mesh). The reactions were performed with a standard 25 mL Schlenk tube equipped with a stir bar and a J. Young valve.

1.2) General analytical information

^1H , ^{13}C and ^{19}F NMR spectra were recorded on a JEOL ECS 400 MHz spectrometer and on a Bruker Avance III 500 MHz spectrometer. All chemical shifts were reported in ppm using tetramethylsilane as a reference. Chemical shifts of ^1H NMR signals are referenced to the indicated residual solvent peak (CDCl_3 , $\delta = 7.26$ ppm). All ^{13}C NMR spectra are reported in ppm relative to CDCl_3 (77.00 ppm) and were obtained with ^1H decoupling. CDCl_3 was obtained from Sigma-Aldrich (Merck). The HRMS data were obtained using a Finnigan MAT 8230 instrument.

2) Experimental Details

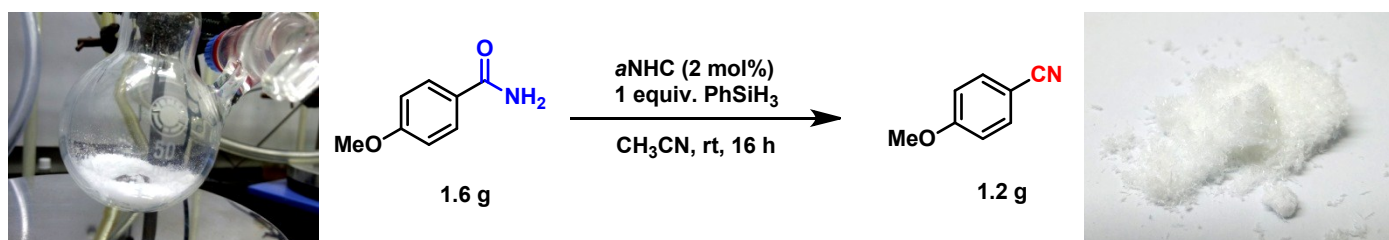
2.1) Experimental procedures for abnormal NHC catalyzed dehydration of primary amides



Scheme S1. General procedure for the dehydration of primary amides to nitriles.

An oven-dried 25mL Schlenk tube was charged with 0.5 mmol amide substrate and a magnetic stirring bar. Amide was kept under high vacuum for 2 h and was transferred into a nitrogen-filled glovebox. Inside the glovebox, abnormal N-heterocyclic carbene (*a*NHC) (2 mol%) and anhydrous acetonitrile (0.6 mL) were added to the reaction tube. The solution was stirred vigorously at room temperature for 2-3 min. While continuously stirring, the appropriate amount of silane (1 equiv.) was added dropwise to the solution using a micropipette. During the addition of silane hydrogen gas evolved in some cases. After that, the tube was sealed tightly with a screw cap equipped with a J. Young valve and removed from the glovebox. The reaction tube was then connected through Schlenk line and stirred at room temperature inside a fume hood for 12 h under nitrogen atmosphere. After 12 h, the reaction tube was uncapped and 2M NaOH solution was added and the organic part was collected in EtOAc. The crude mixture was purified through column chromatography on silica gel (Merck, 100-200 mesh). The corresponding nitrile was identified by ^1H and ^{13}C NMR spectroscopy in CDCl_3 .

2.2) Experimental procedures for gram-scale reaction



Scheme S2. Catalytic dehydration of 4-methoxybenzamide amides to 4-methoxybenzonitrile in gram-scale.

An oven-dried 50mL Schlenk flask was charged with 1.6 g of 4-methoxybenzamide substrate and a magnetic stirring bar. Amide was kept under high vacuum for 3 h and was transferred into a nitrogen-filled glovebox. Inside the glovebox, abnormal N-heterocyclic carbene (*a*NHC) (2 mol%) and anhydrous acetonitrile (22 mL) were added to the reaction tube. The solution was stirred vigorously at room temperature for 10 min. While continuously stirring, the appropriate amount of silane (1 equiv.) was added dropwise to the solution using a micropipette. During the addition of silane, a gas evolution was observed. After that, the flask was closed and removed from the glovebox. The reaction flask was then connected through Schlenk line and stirred at room temperature inside a fume hood for 16 h under nitrogen atmosphere. After 16 h, the reaction tube was opened and 2M NaOH solution was added and the organic part was collected in EtOAc. The crude mixture was purified through column chromatography on silica gel (Merck, 100-200 mesh). The corresponding nitrile was identified by ¹H and ¹³C NMR spectroscopy in CDCl₃. Yield of the product is 85%.

2.3) Conversion vs time plot

We monitored the progress of the dehydration reaction by looking at the conversion vs. time graph for 4-methoxybenzamide substrate with catalyst *a*NHC as shown in Fig. S1. The

reaction was carried out at room temperature for 12 h with 4-methoxybenzamide and phenylsilane in presence of 2 mol% catalyst loading. The yield of the product was 60% after 3 h, and within 5 h, it furnishes a satisfactory yield, 91 % at room temperature. Finally, within 6 h, the reaction reaches near resulting in 99% conversion (Fig. S1).

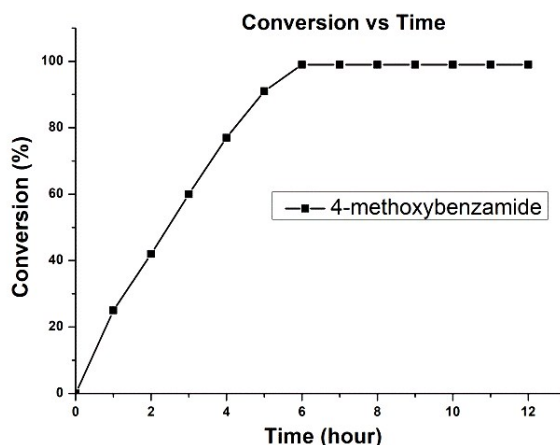
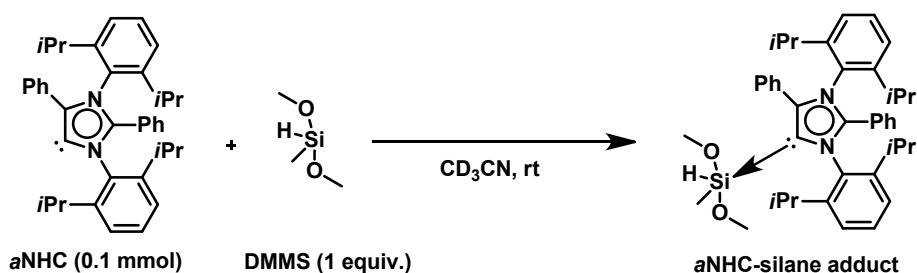


Fig. S1 Plot of conversion (%) versus time (hour) in the dehydration of 4-methoxybenzamide (0.3 mmol) and phenylsilane (0.3 mmol) catalyzed by *a*NHC (2 mol %).

2.4) Characterization of the reaction intermediate *a*NHC-silane adduct



Scheme S3. Stoichiometric reaction of *a*NHC and DMMS at room temperature.

Under an argon atmosphere, a 2.5 mL screw cap NMR tube was charged with *a*NHC (0.1 mmol), and DMMS (1 equiv.) in acetonitrile- d_3 (0.6 mL). ^{29}Si NMR spectrum was then recorded in acetonitrile- d_3 solvent.

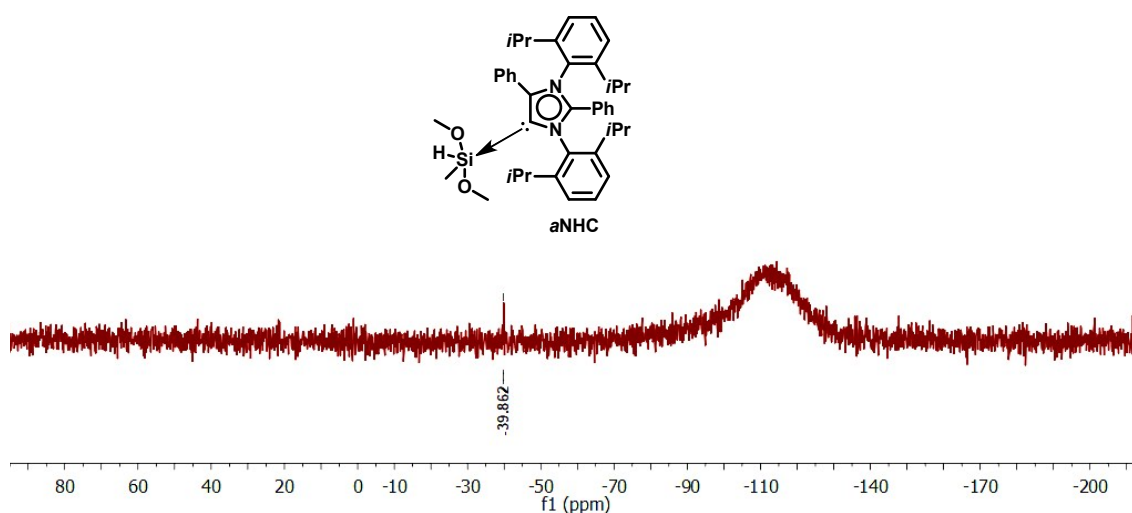
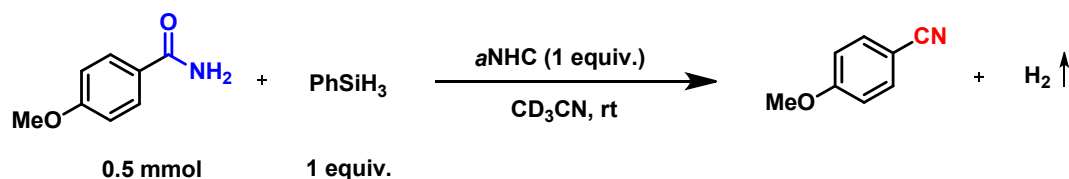


Fig. S2. ^{29}Si NMR spectrum of *a*NHC-silane adduct in acetonitrile- d_3 (DMMS was used as a silane source) displaying a peak at $\delta = -39.9$ ppm which appears at high shielded zone compare to free silane ($\delta = -13.0$ ppm).

2.5) H_2 evolution experiment



Scheme S4. Stoichiometric reaction of amide, silane and *a*NHC in acetonitrile- d_3 at room temperature.

Under an argon atmosphere, a 2.5 mL screw cap NMR tube was charged with 4-methoxybenzamide (7.55 mg), *a*NHC (1 equiv.), phenylsilane (1 equiv.) and acetonitrile- d_3 (0.6 mL). During the addition of phenylsilane at room temperature, we observed a gas evolution which was confirmed as hydrogen from ^1H NMR ($\delta = 4.57$ ppm) spectrum.¹

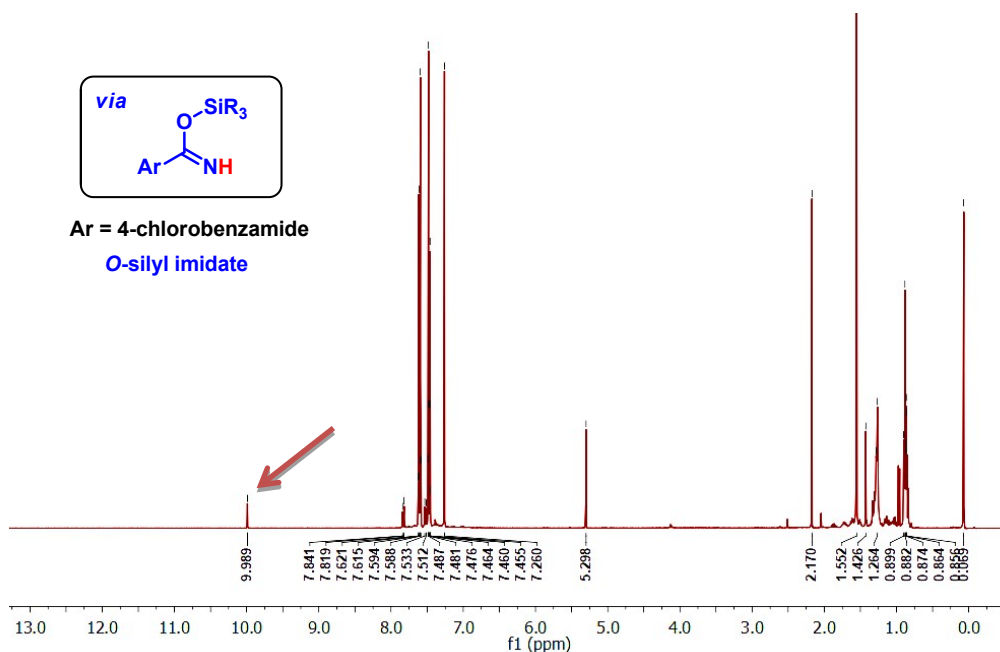


Fig. S4 Reaction mixture of catalytic silylative dehydration of 4-chlorobenzamide with phenylsilane in CDCl_3 where the peak at $\delta = 9.98$ ppm indicating the imine proton.

2.7) Control experiment using a model imine, benzophenone imine and *a*NHC in acetonitrile- d_3 solvent

Under an argon atmosphere, a 2.5 mL screw cap NMR tube was charged with benzophenone imine (0.1 mmol) and *a*NHC (0.1 mmol) in acetonitrile- d_3 solvent and ^1H NMR spectrum was recorded. After addition of *a*NHC, the benzophenone imine peak at δ 9.93 ppm disappeared indicating a hydrogen bonding interaction between free carbene and benzophenone imine.

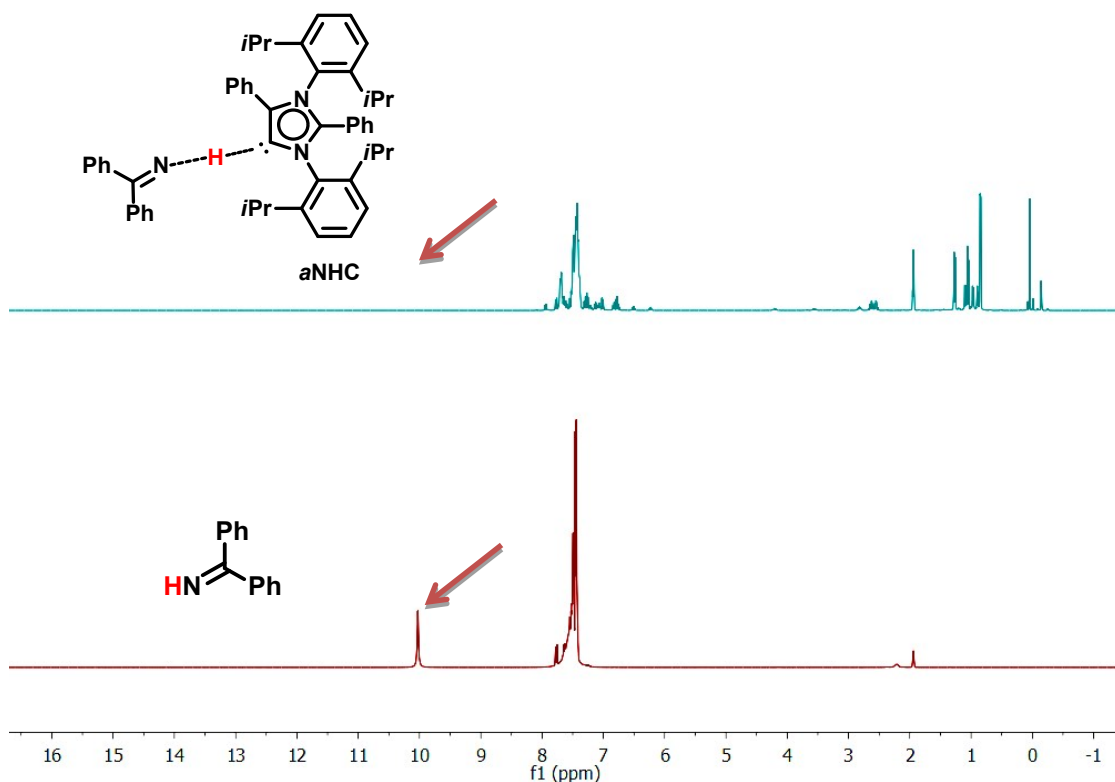
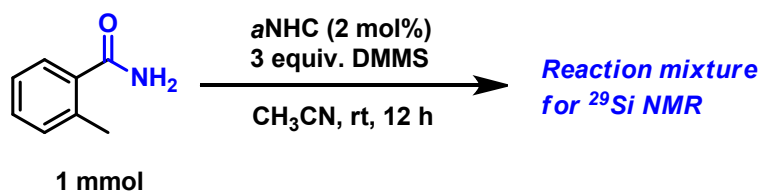


Fig. S5 ^1H NMR spectrum of benzophenone imine in acetonitrile- d_3 (bottom) displaying the imine peak at δ 9.93 ppm. ^1H NMR spectrum of the reaction mixture (benzophenone imine and *a*NHC in acetonitrile- d_3) displaying the absence of the imine peak at δ 9.93 ppm (top).

2.8) Characterization of the silicon byproduct

An oven-dried 25mL Schlenk tube was charged with 1 mmol 2-methylbenzamide substrate and a magnetic stirring bar. Amide was kept under high vacuum for 2 h and was transferred into a nitrogen-filled glovebox. Inside the glovebox, abnormal N-heterocyclic carbene



Scheme S6. Catalytic dehydration reaction mixture where DMMS was used as a silane.

(*a*NHC) catalyst (2 mol%) and anhydrous acetonitrile (0.6 mL) were added to the reaction tube. The solution was stirred vigorously at room temperature for 2-3 min. While continuously stirring, the appropriate amount of DMMS (3 equiv.) was added dropwise to the solution using a micropipette. After that, the tube was sealed tightly with a screw cap equipped with a J. Young valve and removed from the glovebox. The reaction tube was then

connected through Schlenk line and stirred at room temperature inside a fume hood for 12 h under nitrogen atmosphere. After 12 h, the reaction tube was uncapped and ^{29}Si NMR spectrum was recorded of the crude mixture in CDCl_3 .

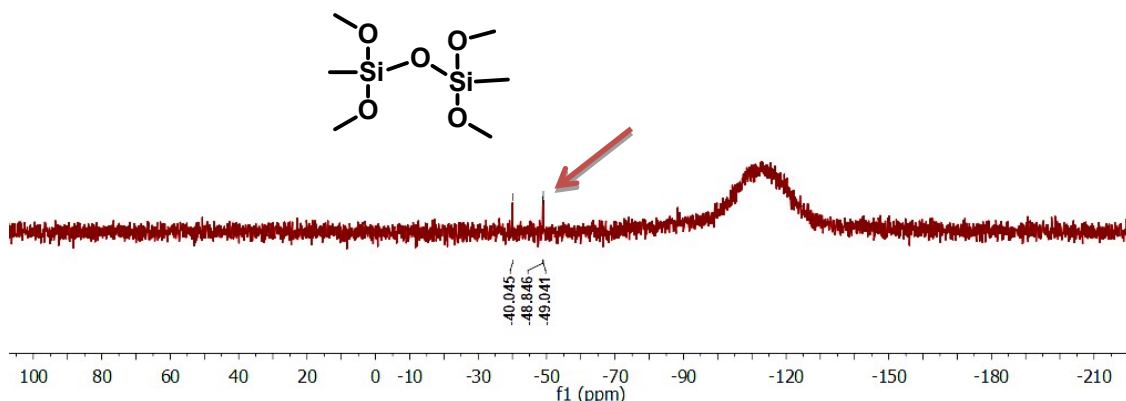
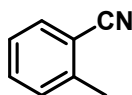


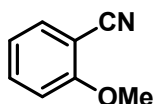
Fig. S6 ^{29}Si NMR spectrum of the catalytic reaction mixture in CDCl_3 where the peak at -49.0 ppm may be attributed to ^{29}Si nuclei of siloxane by comparing the previous reported value.²

3) Characterization

3.1) ^1H , ^{13}C and ^{19}F NMR Data of Nitrile Products

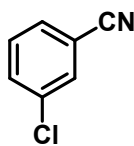


2-Methylbenzonitrile (**2a**)³: ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): δ = 7.51 (d, J = 8.0 Hz, 1H), 7.41 (t, J = 7.6 Hz, 1H), 7.26-7.18 (m, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): δ = 141.6, 132.4, 132.2, 130.0, 126.0, 117.9, 112.5, 20.2. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.

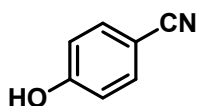


2-Methoxybenzonitrile (**2b**)³: ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): δ = 7.55-7.51 (m, 2H), 7.01-6.95 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3 , 25 °C, TMS): δ = 161.1,

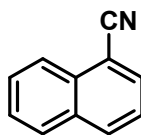
134.3, 133.6, 120.7, 116.4, 111.2, 101.7, 55.9. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



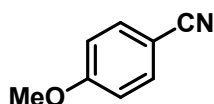
3-Chlorobenzonitrile (**2c**)⁴: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.64-7.63 (m, 1H), 7.59-7.55 (m, 2H), 7.43 (t, *J* = 8.0 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 135.2, 133.2, 131.9, 130.4, 130.3, 117.4, 113.9. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



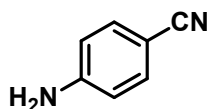
4-Hydroxybenzonitrile (**2d**)⁴: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.54 (d, *J* = 8.8 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 160.3, 134.3, 119.2, 116.5, 102.8. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (88 : 12 v/v) as eluent.



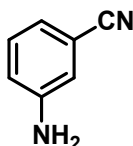
1-Naphthonitrile (**2e**)⁵: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 8.18 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 2H), 7.66-7.62 (m, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 133.2, 132.8, 132.5, 132.2, 128.5, 128.4, 127.4, 124.9, 124.8, 117.7, 110.0. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



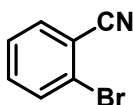
4-Methoxybenzonitrile (**2f**)⁶: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.55 (d, J = 8.8 Hz, 2H), 6.92 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 162.7, 133.8, 119.1, 114.6, 103.8, 55.4. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



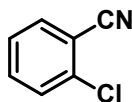
4-Aminobenzonitrile (**2g**)⁵: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.38 (d, J = 8.4 Hz, 2H), 6.63 (d, J = 8.8 Hz, 2H), 4.23 (bs, 2H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 150.5, 133.7, 120.1, 114.3, 99.7. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (82 : 18 v/v) as eluent.



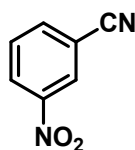
3-Aminobenzonitrile (**2h**)⁷: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.21 (t, J = 8.0 Hz, 1H), 7.00 (d, J = 7.6 Hz, 1H), 6.89-6.84 (m, 2H), 3.88 (bs, 2H); ¹³C NMR (125 MHz, CDCl₃, 25 °C, TMS): δ = 147.0, 129.9, 121.6, 119.2, 119.1, 117.2, 112.6. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (82 : 18 v/v) as eluent.



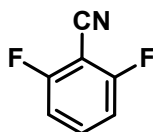
2-Bromobenzonitrile (**2i**)⁸: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.69-7.64 (m, 2H), 7.48-7.40 (m, 2H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 134.2, 133.8, 133.1, 127.6, 125.2, 117.1, 115.8. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



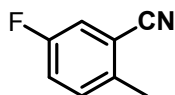
2-Chlorobenzonitrile (**2j**)⁸: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.69-7.66 (m, 1H), 7.55-7.52 (m, 2H), 7.39-7.35 (m, 1H); ¹³C NMR (125 MHz, CDCl₃, 25 °C, TMS): δ = 136.9, 134.0, 133.8, 130.0, 127.1, 115.9, 113.5. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



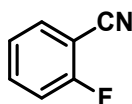
3-Nitrobenzonitrile (**2k**): ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 8.51-8.40 (m, 2H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 8.0 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃, 25 °C, TMS): δ = 148.3, 137.5, 130.6, 127.5, 127.2, 116.5, 114.2. ESI-MS: *m/z*: [M+H]⁺ calculated for C₇H₅N₂O₂ 149.0351; found 149.0252. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (95 : 5 v/v) as eluent.



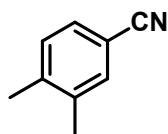
2,6-Difluorobenzonitrile (**2l**): ^1H NMR (500 MHz, CDCl_3 , 25 °C, TMS): δ = 7.64-7.58 (m, 1H), 7.06 (t, J = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, CDCl_3 , 25 °C, TMS): δ = 164.4, 164.3, 162.3, 135.6, 135.5, 135.4, 112.2, 112.2, 112.1, 112.0, 109.1, 92.6; ^{19}F NMR (470 MHz, CDCl_3 , 25 °C, TMS): δ = -103.5. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



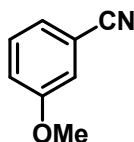
5-Fluoro-2-methylbenzonitrile (**2m**)³: ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): δ = 7.26-7.22 (m, 2H), 7.17-7.12 (m, 1H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3 , 25 °C, TMS): δ = 161.2, 159.3, 137.9, 137.8, 131.9, 131.9, 120.3, 120.1, 118.9, 118.8, 116.9, 116.8, 113.8, 113.7, 19.6; ^{19}F NMR (470 MHz, CDCl_3 , 25 °C, TMS): δ = -115.2. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



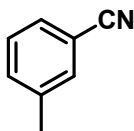
2-Fluorobenzonitrile (**2n**)⁹: ^1H NMR (400 MHz, CDCl_3 , 25 °C, TMS): δ = 7.63-7.58 (m, 2H), 7.28-7.19 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3 , 25 °C, TMS): δ = 164.1, 162.1, 135.0, 134.9, 133.5, 124.8, 124.8, 116.5, 116.4, 113.9, 101.6, 101.5; ^{19}F NMR (470 MHz, CDCl_3 , 25 °C, TMS): δ = -106.2. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



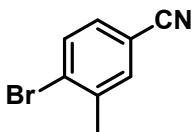
3,4-Dimethylbenzonitrile (**2o**)¹⁰: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.37-7.35 (m, 2H), 7.19 (d, J = 7.6 Hz, 1H), 2.30 (s, 3H), 2.27 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 142.4, 137.8, 132.7, 130.2, 129.5, 119.2, 109.4, 19.9, 19.4. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



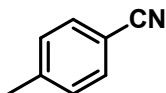
3-Methoxybenzonitrile (**2p**)³: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.38-7.34 (m, 1H), 7.23 (d, J = 7.6 Hz, 1H), 7.13-7.11 (m, 2H), 3.83 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 159.7, 130.4, 124.5, 119.4, 118.8, 116.9, 113.2, 55.6. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



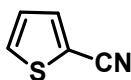
3-Methylbenzonitrile (**2q**)¹¹: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.45-7.43 (m, 2H), 7.41-7.39 (m, 1H), 7.36-7.32 (m, 1H), 2.38 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 139.2, 133.6, 132.4, 129.2, 128.9, 118.9, 112.2, 21.1. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



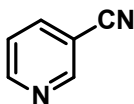
4-Bromo-3-methylbenzonitrile (**2r**)¹²: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.63 (d, J = 8.0 Hz, 1H), 7.50 (s, 1H), 7.33-7.30 (m, 1H), 2.43 (s, 3H); ¹³C NMR (125 MHz, CDCl₃, 25 °C, TMS): δ = 139.6, 133.8, 133.3, 130.5, 130.4, 118.1, 111.3, 22.8. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



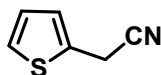
4-Methylbenzonitrile (**2s**)¹¹: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.51 (d, J = 8.0 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 143.6, 131.9, 129.7, 119.1, 109.2, 21.7. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



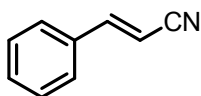
Thiophene-2-carbonitrile (**2t**)⁶: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.64-7.60 (m, 2H), 7.15-7.13 (m, 1H); ¹³C NMR (125 MHz, CDCl₃, 25 °C, TMS): δ = 137.4, 132.5, 127.6, 114.2, 109.9. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



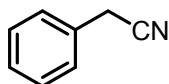
Nicotinonitrile (**2u**)⁶: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 8.90-8.82 (m, 2H), 7.98-7.96 (m, 1H), 7.46-7.43 (m, 1H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 152.9, 152.4, 139.2, 123.6, 116.4, 110.1. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (80 : 20 v/v) as eluent.



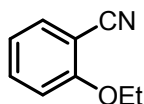
2-(Thiophen-2-yl)acetonitrile (**2v**)¹³: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.27-7.26 (m, 1H), 7.06-7.05 (m, 1H), 6.99-6.97 (m, 1H), 3.90 (s, 3H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 130.9, 127.2, 127.1, 125.8, 116.9, 18.5. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



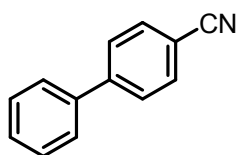
Cinnamionitrile (**2aa**)¹¹: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.45-7.37 (m, 6H), 5.87 (d, J = 16.8 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 150.4, 133.4, 131.1, 129.0, 127.2, 118.1, 96.2. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



2-Phenylacetonitrile (**2ab**)⁶: ¹H NMR (400 MHz, CDCl₃, 25 °C, TMS): δ = 7.41-7.32 (m, 5H), 3.72 (s, 2H); ¹³C NMR (100 MHz, CDCl₃, 25 °C, TMS): δ = 129.8, 128.9, 127.8, 127.7, 117.8, 23.3. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



2-Ethoxybenzonitrile (**2ac**): ^1H NMR (400 MHz, CDCl_3 , 25 $^\circ\text{C}$, TMS): δ = 7.49-7.45 (m, 2H), 6.96-6.91 (m, 2H), 4.10 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3 , 25 $^\circ\text{C}$, TMS): δ = 160.4, 134.2, 133.5, 120.4, 116.4, 112.0, 101.7, 64.4, 14.3. ESI-MS: m/z : $[\text{M}+\text{Na}]^+$ calculated for $\text{C}_9\text{H}_9\text{NONa}$ 170.0582; found 170.0576. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.



[1,1'-Biphenyl]-4-carbonitrile (**2ad**)¹⁴: ^1H NMR (400 MHz, CDCl_3 , 25 $^\circ\text{C}$, TMS): δ = 7.72-7.66 (m, 4H), 7.60-7.58 (m, 2H), 7.51-7.43 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3 , 25 $^\circ\text{C}$, TMS): δ = 145.4, 138.9, 132.4, 128.9, 128.5, 127.5, 127.0, 118.8, 110.7. The compound was purified by column chromatography on silica gel with hexane and ethyl acetate mixture (98 : 2 v/v) as eluent.

3.2) ^1H and ^{13}C NMR Spectra of Nitrile Products

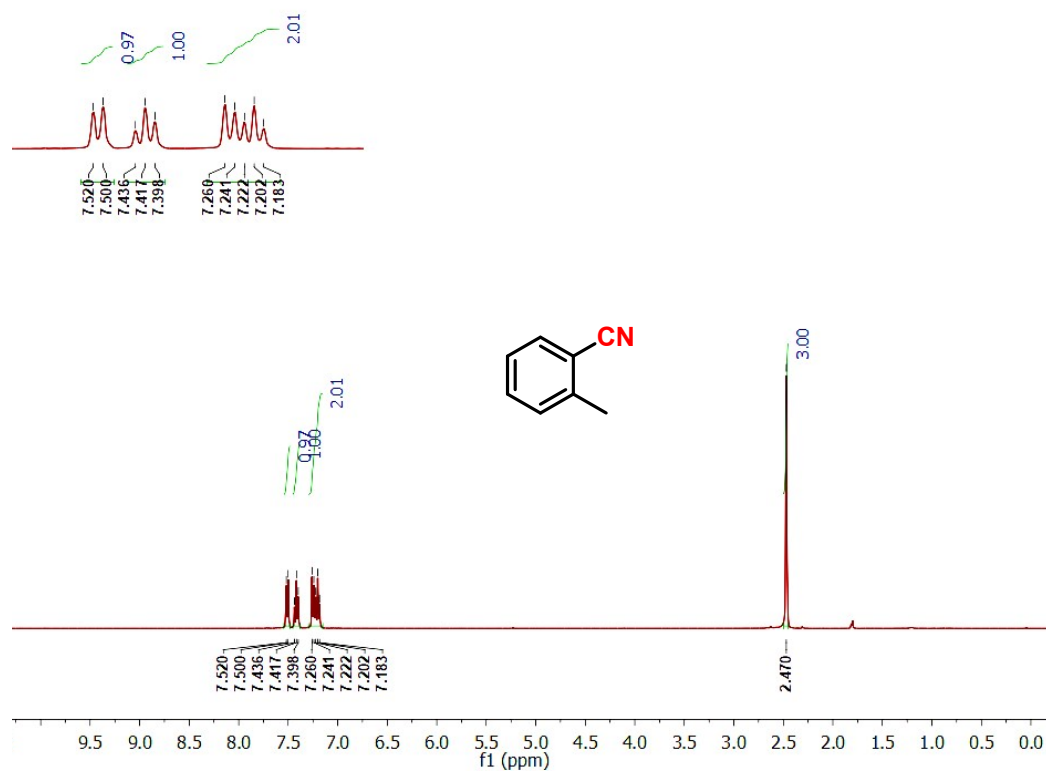


Fig. S7 ^1H NMR (in CDCl_3) spectrum of 2-methylbenzonitrile (**2a**).³

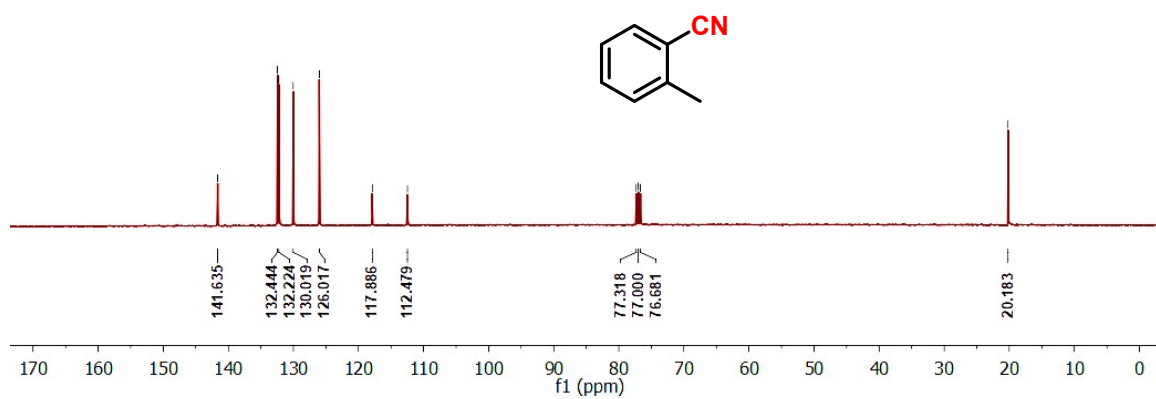


Fig. S8 ^{13}C NMR (in CDCl_3) spectrum of 2-methylbenzonitrile (**2a**).³

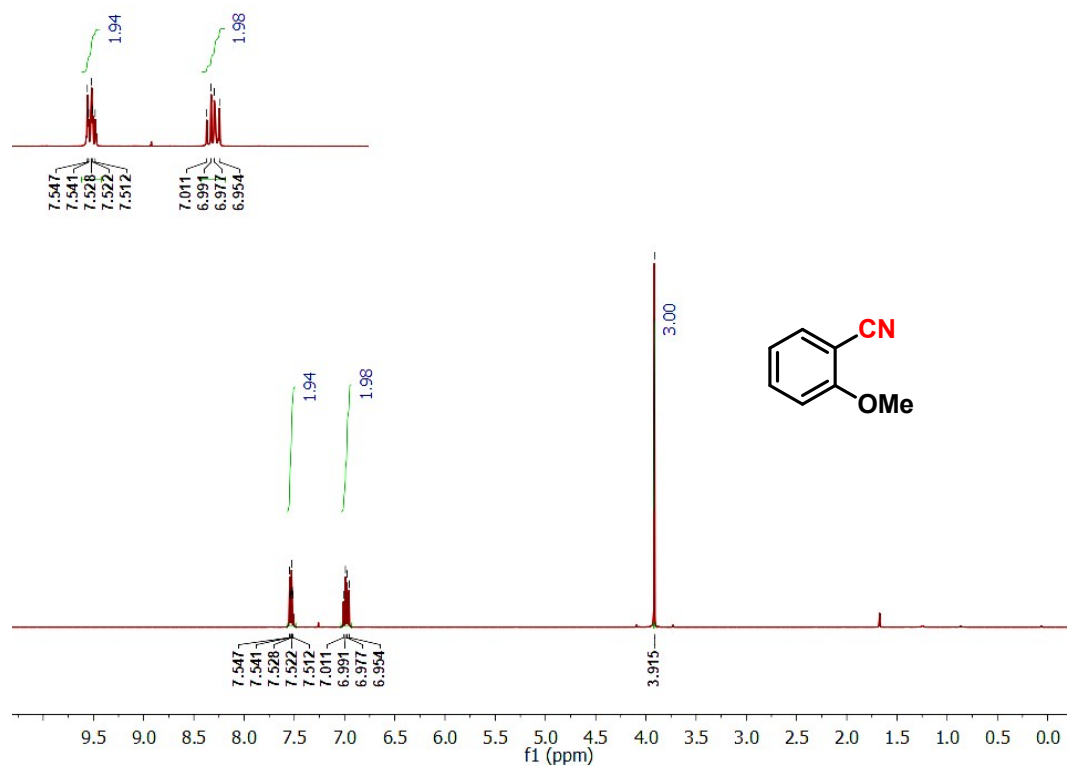


Fig. S9 ¹H NMR (in CDCl₃) spectrum of 2-methoxybenzonitrile (**2b**).³

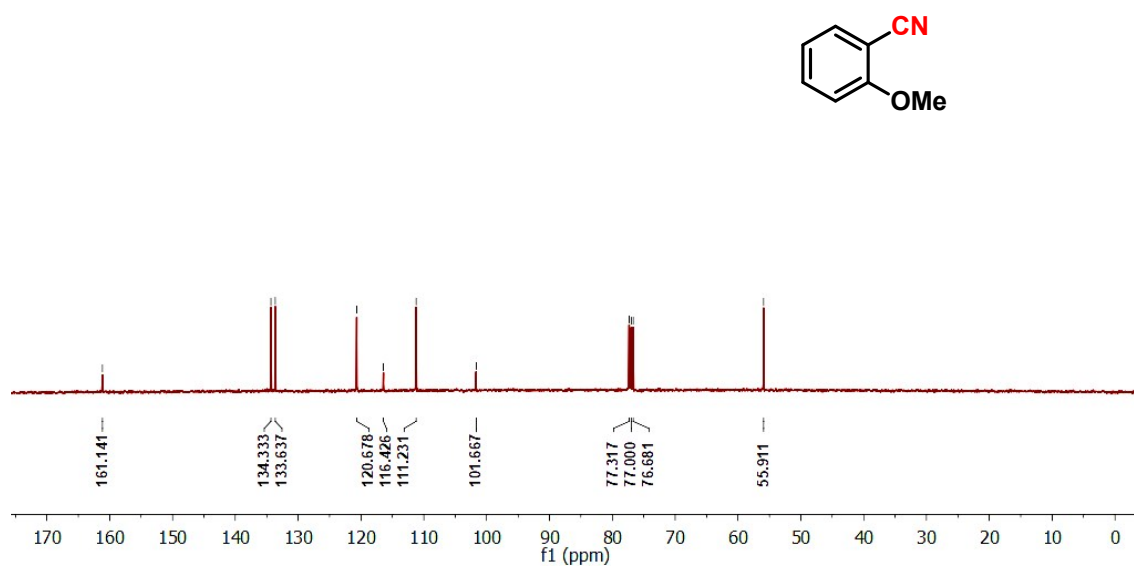


Fig. S10 ¹³C NMR (in CDCl₃) spectrum of 2-methoxybenzonitrile (**2b**).³

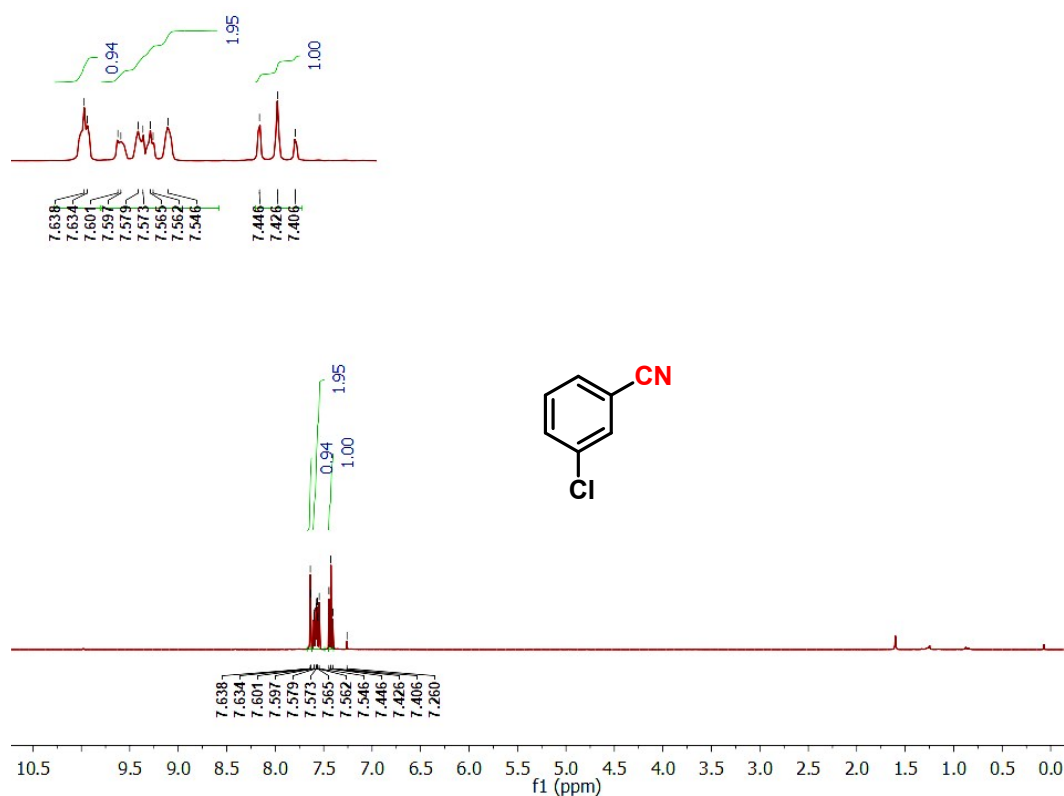


Fig. S11 ¹H NMR (in CDCl₃) spectrum of 3-chlorobenzonitrile (**2c**).⁴

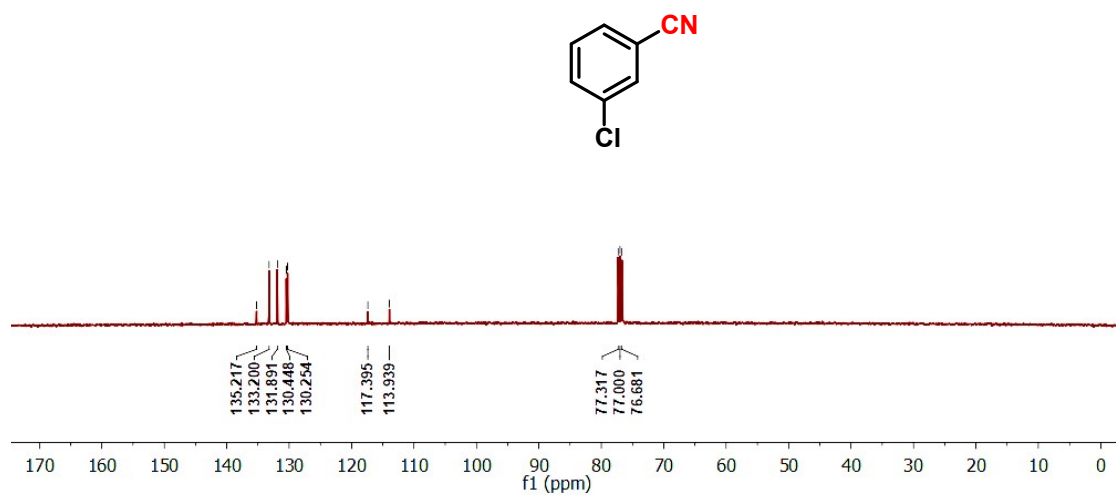


Fig. S12 ¹³C NMR (in CDCl₃) spectrum of 3-chlorobenzonitrile (**2c**).⁴

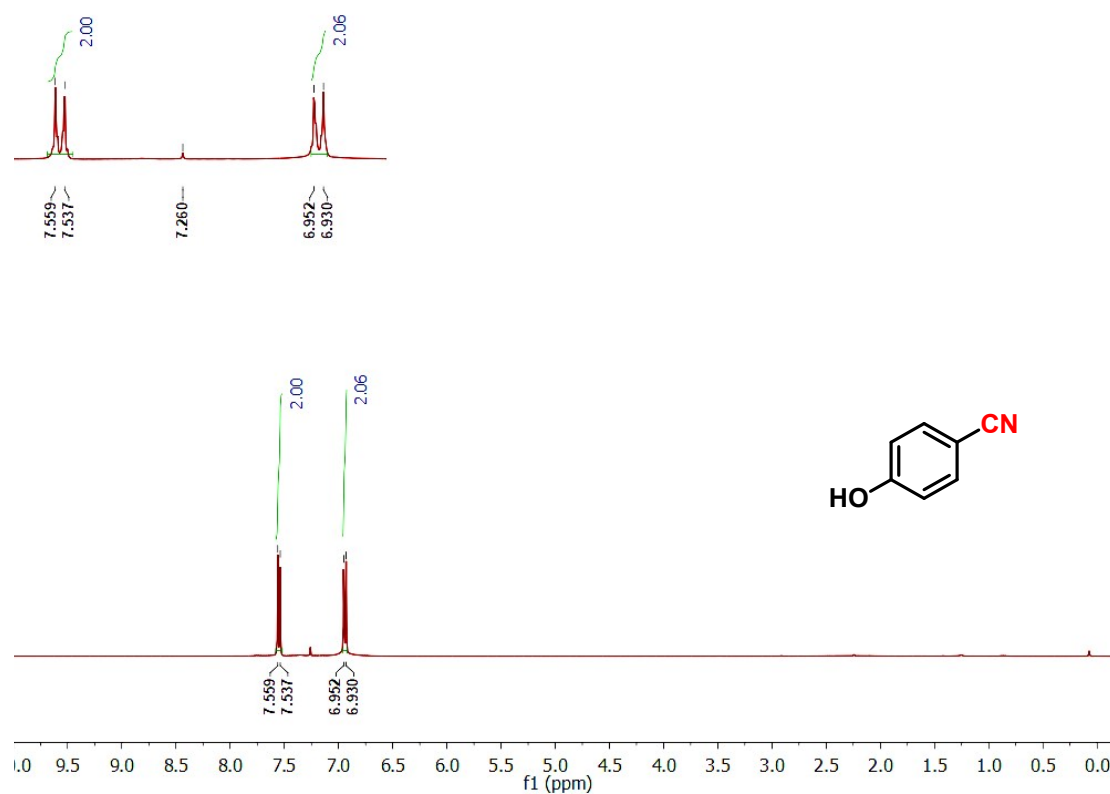


Fig. S13 ¹H NMR (in CDCl₃) spectrum of 4-hydroxybenzonitrile (**2d**).⁴

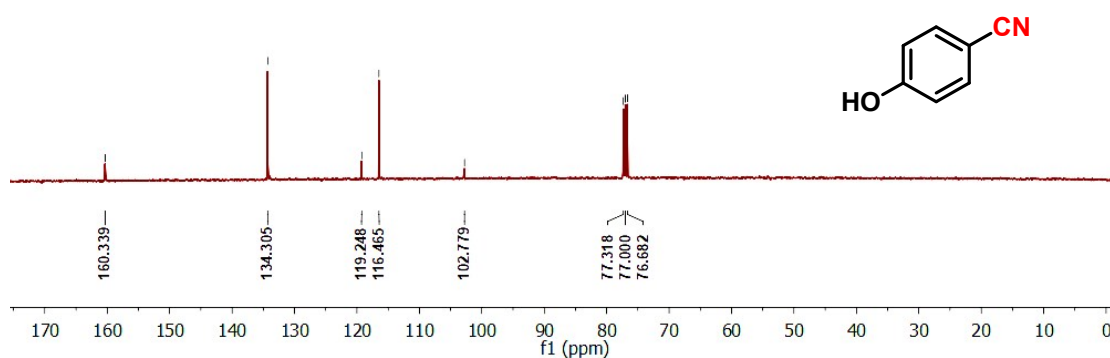


Fig. S14 ¹³C NMR (in CDCl₃) spectrum of 4-hydroxybenzonitrile (**2d**).⁴

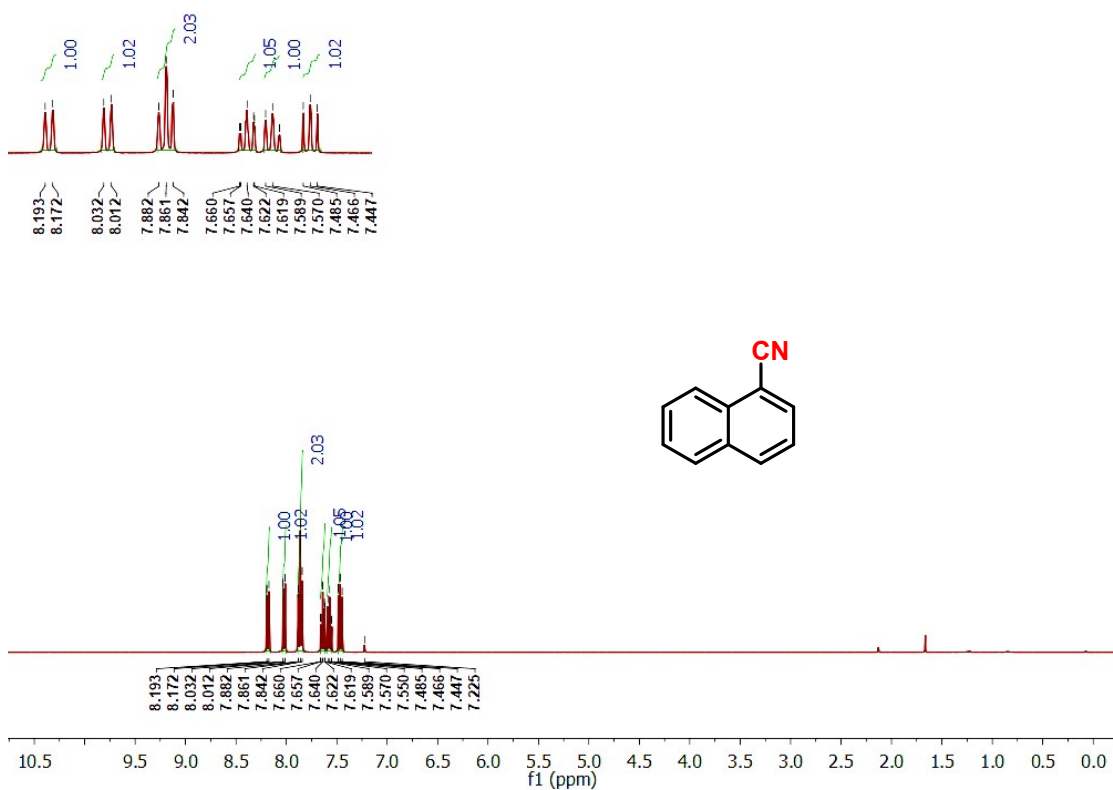


Fig. S15 ¹H NMR (in CDCl₃) spectrum of 1-naphthonitrile (**2e**).⁵

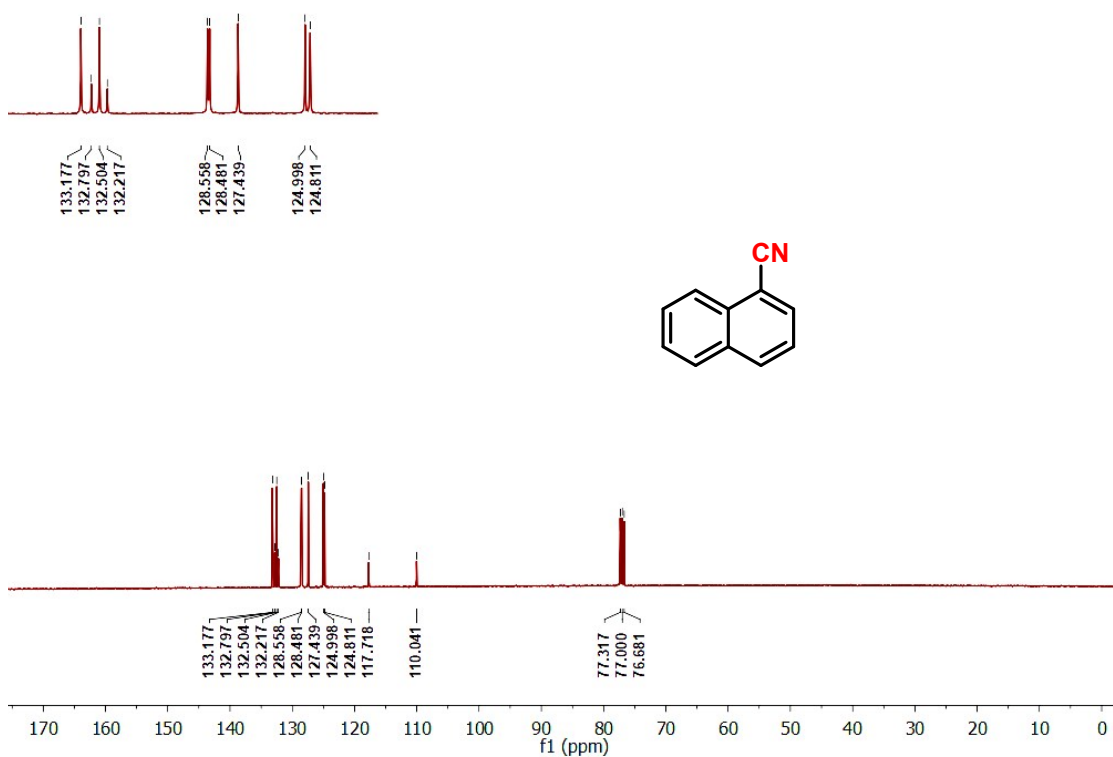


Fig. S16 ¹³C NMR (in CDCl₃) spectrum of 1-naphthonitrile (**2e**).⁵

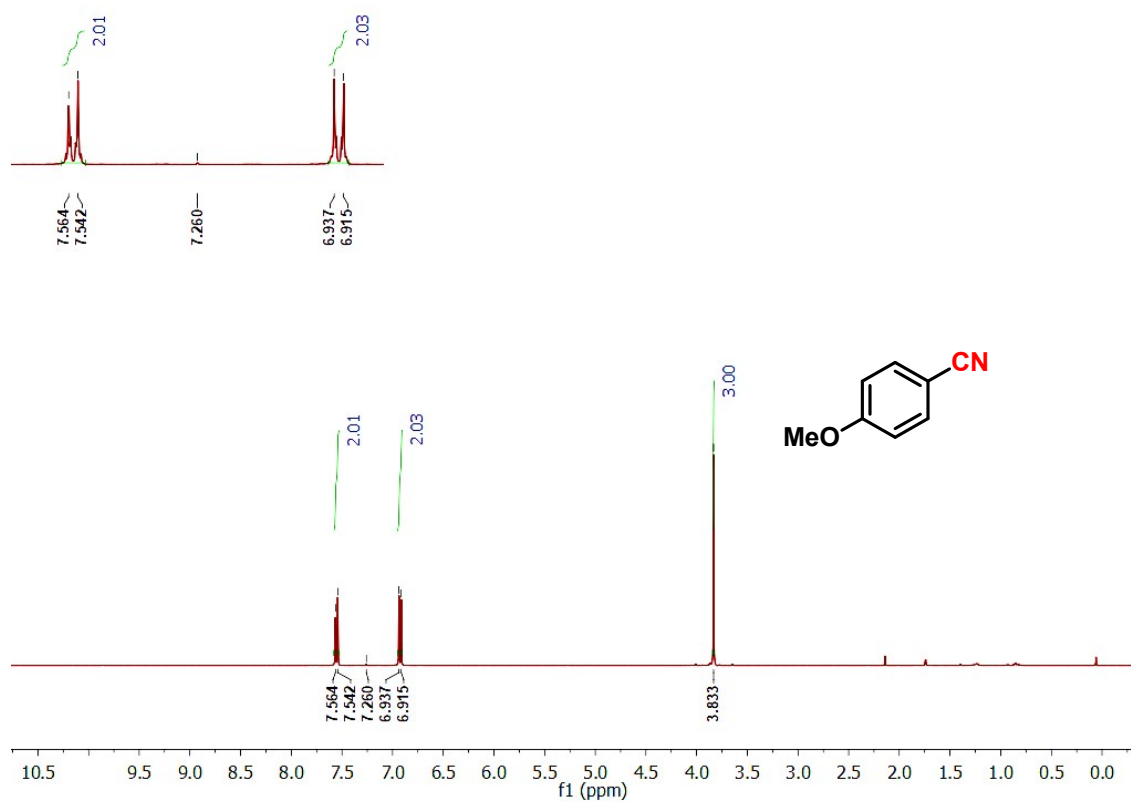


Fig. S17 ¹H NMR (in CDCl₃) spectrum of 4-methoxybenzonitrile (**2f**).⁶

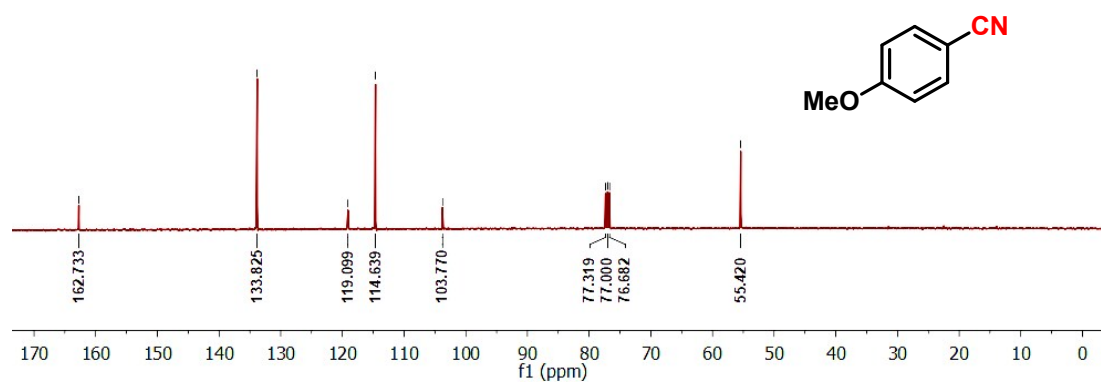


Fig. S18 ¹³C NMR (in CDCl₃) spectrum of 4-methoxybenzonitrile (**2f**).⁶

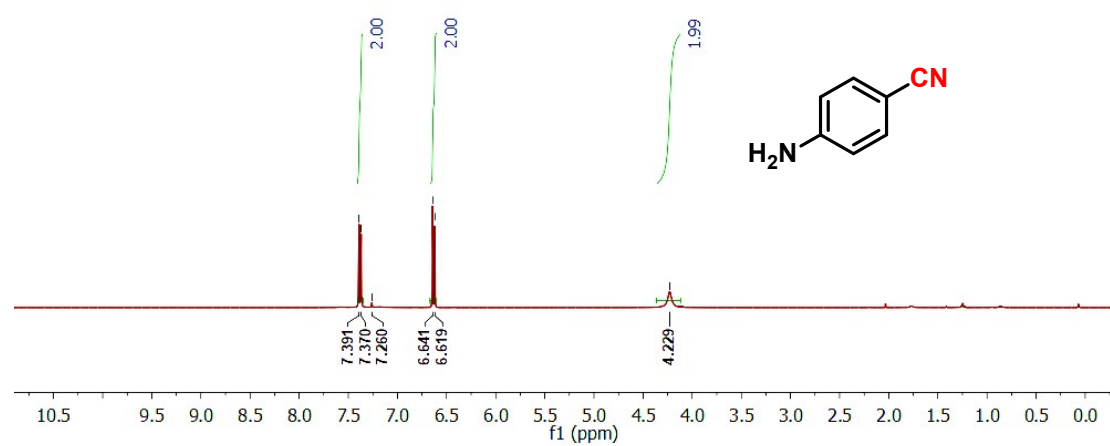


Fig. S19 ¹H NMR (in CDCl₃) spectrum of 4-aminobenzonitrile (**2g**).⁵

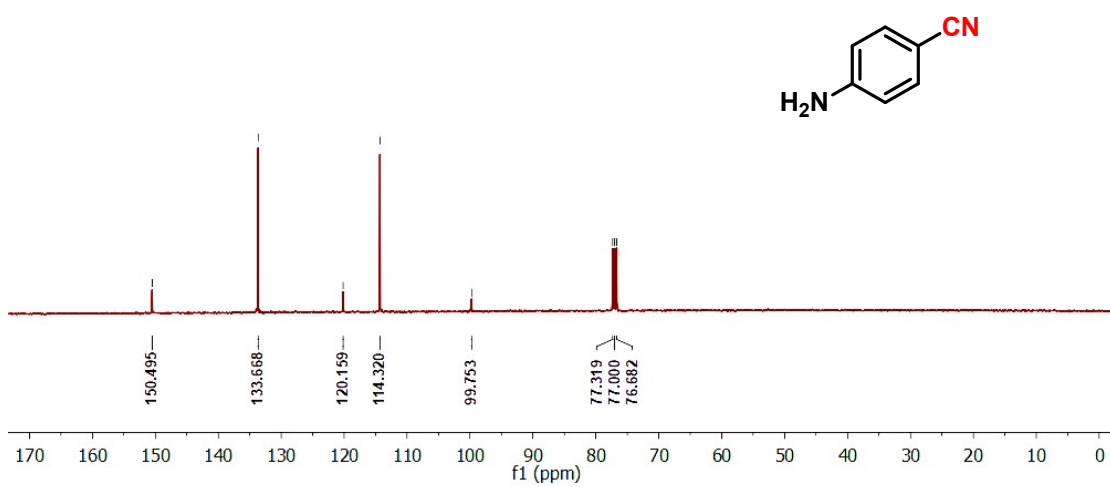


Fig. S20 ¹³C NMR (in CDCl₃) spectrum of 4-aminobenzonitrile (**2g**).⁵

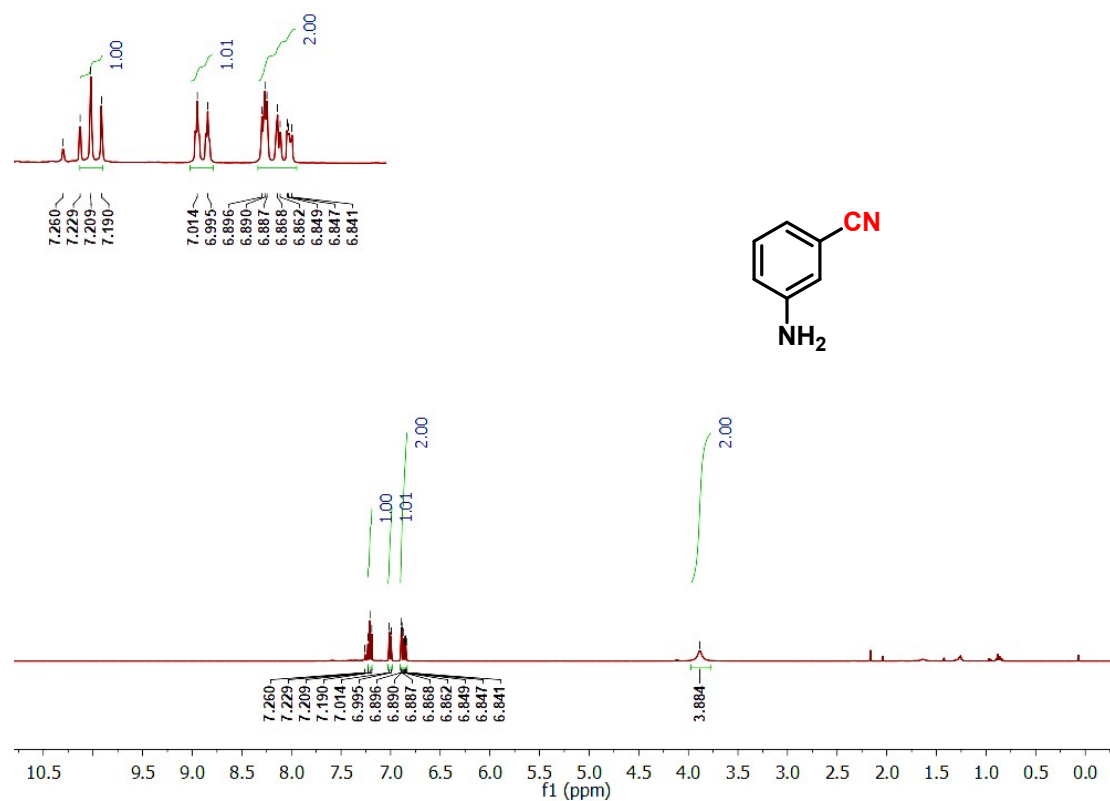


Fig. S21 ¹H NMR (in CDCl₃) spectrum of 3-aminobenzonitrile (**2h**).⁷

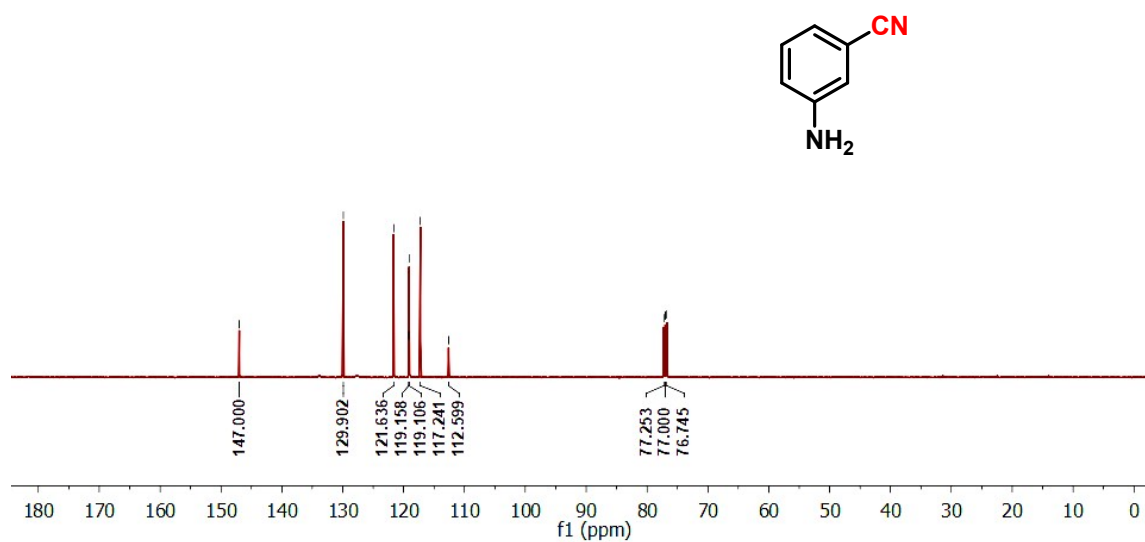


Fig. S22 ¹³C NMR (in CDCl₃) spectrum of 3-aminobenzonitrile (**2h**).⁷

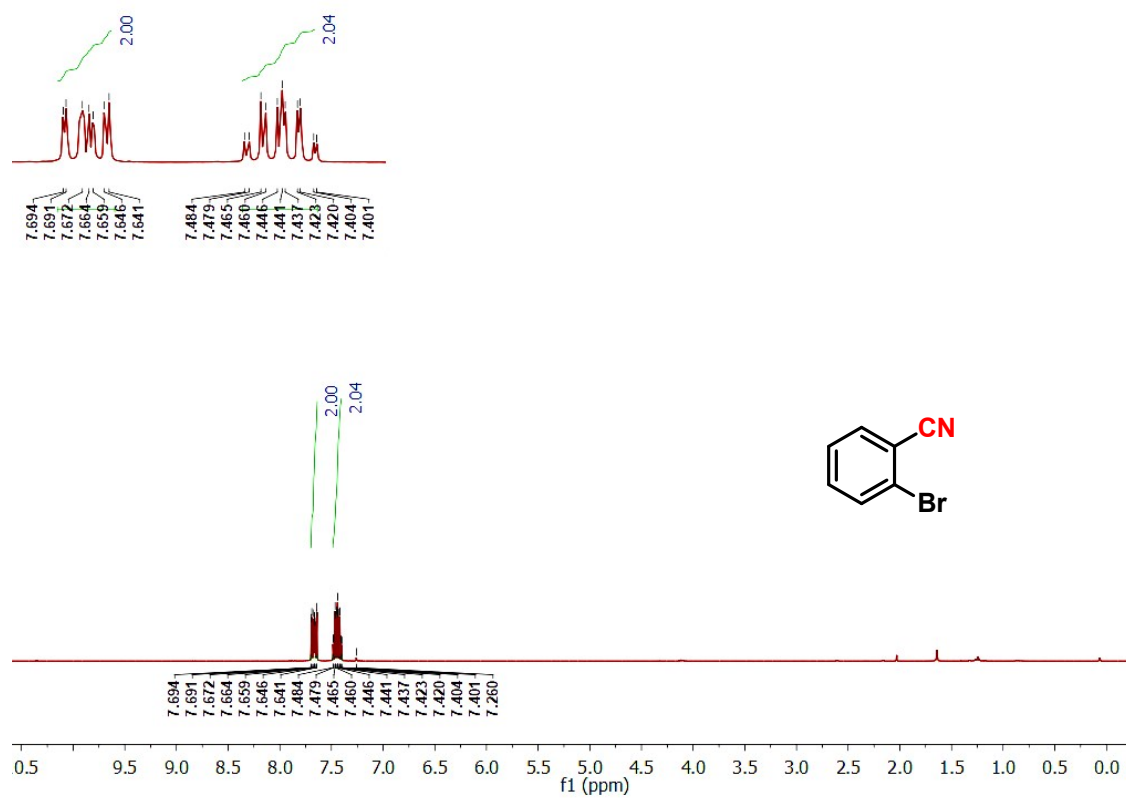


Fig. S23 ¹H NMR (in CDCl₃) spectrum of 2-bromobenzonitrile (**2i**).⁸

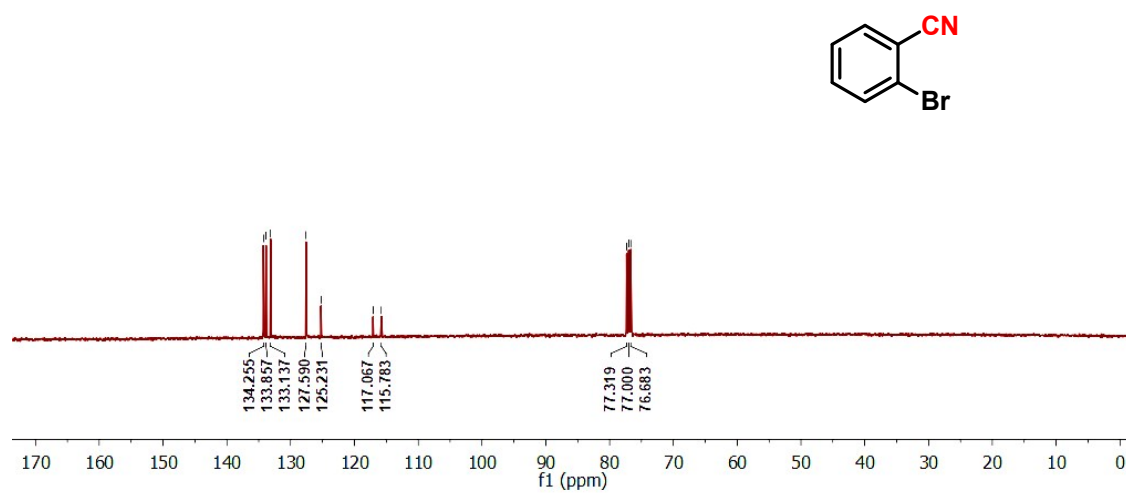


Fig. S24 ¹³C NMR (in CDCl₃) spectrum of 2-bromobenzonitrile (**2i**).⁸

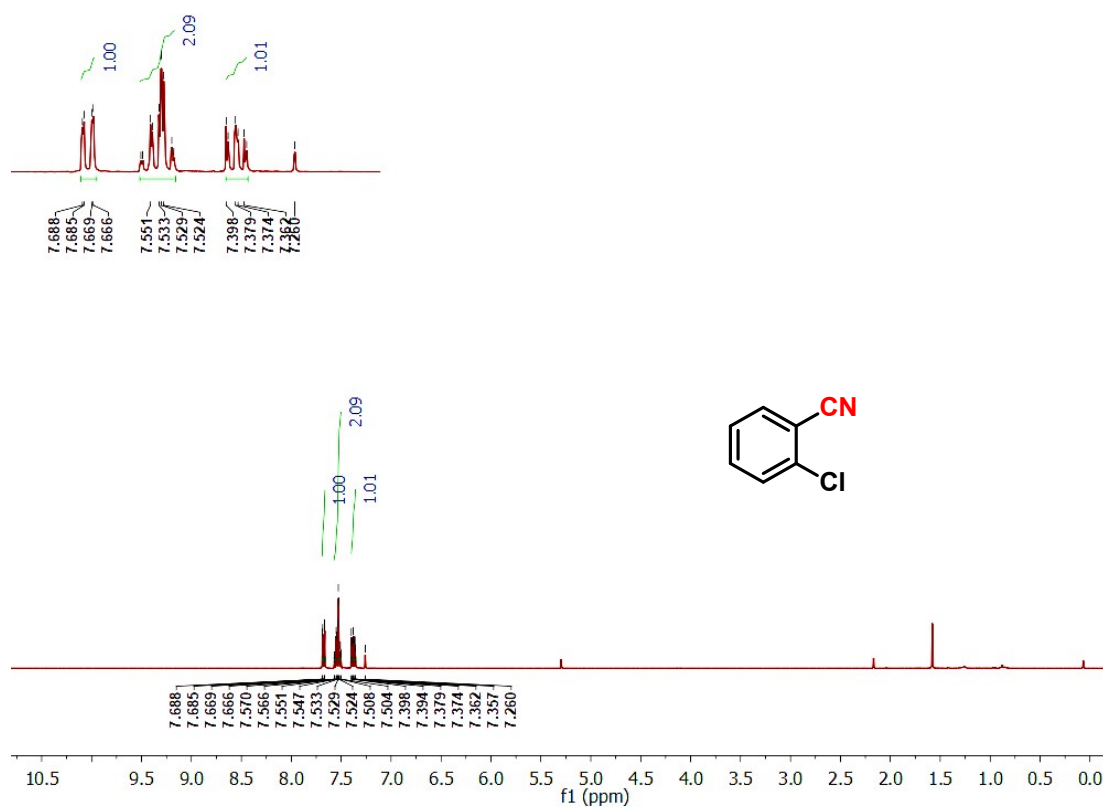


Fig. S25 ¹H NMR (in CDCl₃) spectrum of 2-chlorobenzonitrile (**2j**).⁸

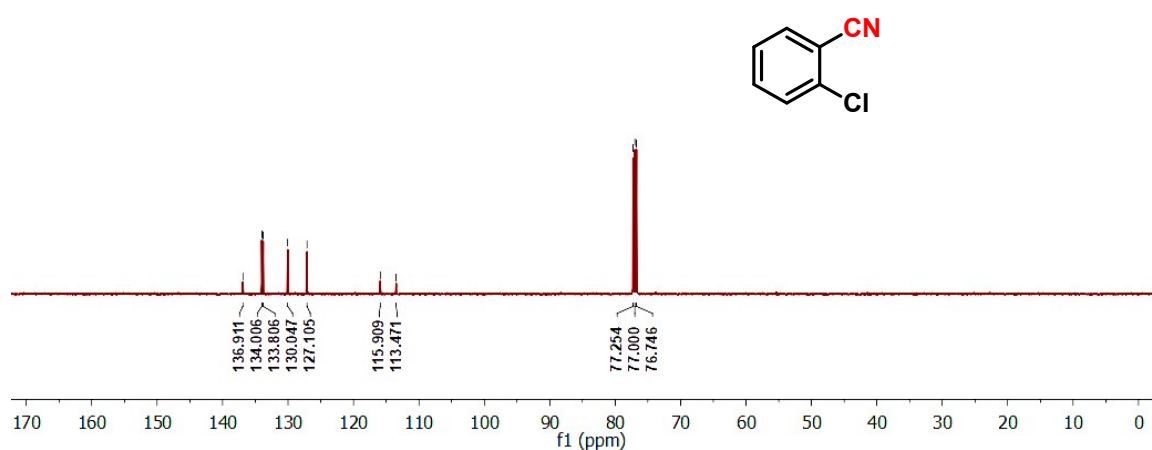


Fig. S26 ¹³C NMR (in CDCl₃) spectrum of 2-chlorobenzonitrile (**2j**).⁸

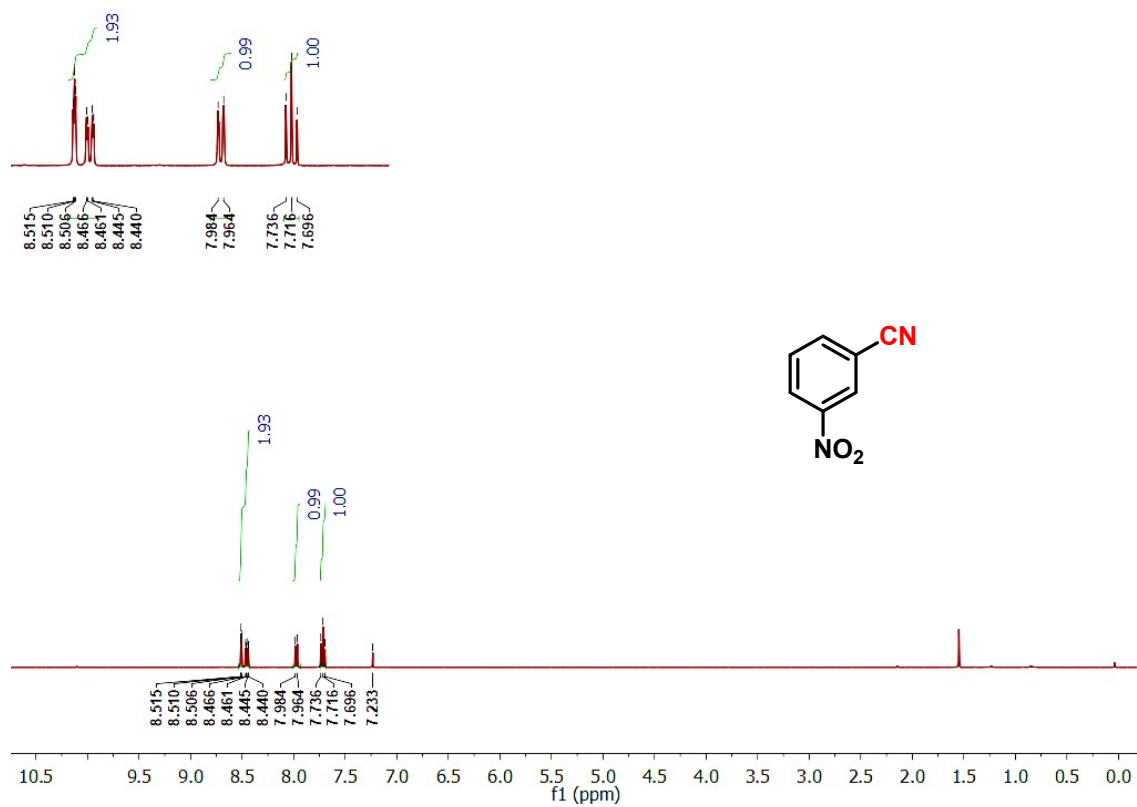


Fig. S27 ¹H NMR (in CDCl₃) spectrum of 3-nitrobenzonitrile (**2k**).

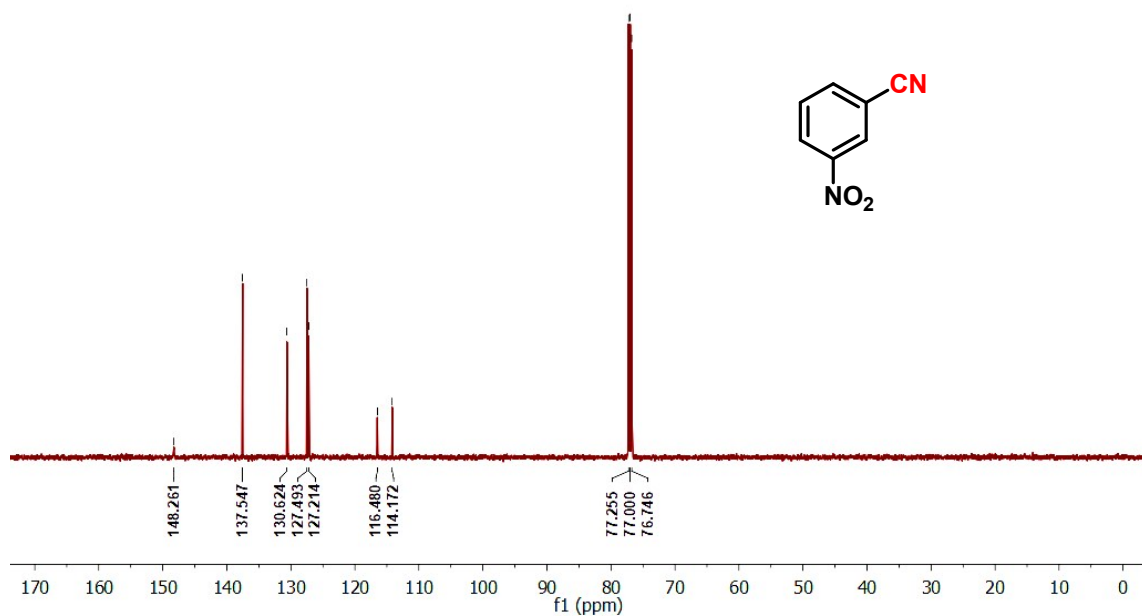


Fig. S28 ¹³C NMR (in CDCl₃) spectrum of 3-nitrobenzonitrile (**2k**).

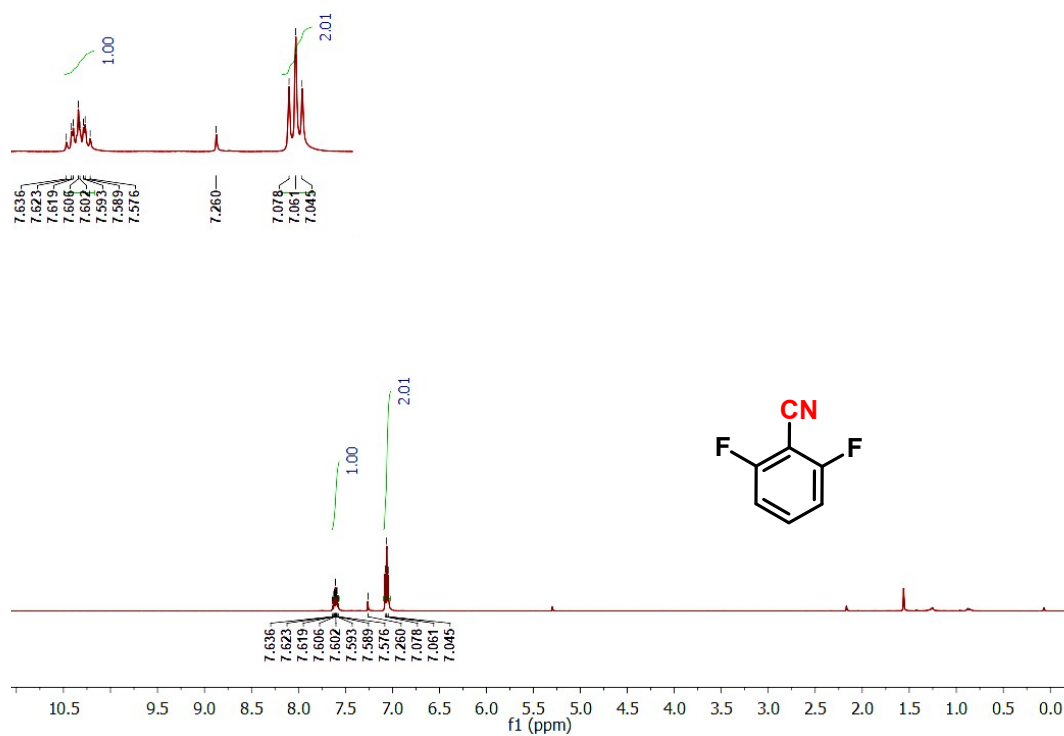


Fig. S29 ¹H NMR (in CDCl₃) spectrum of 2,6-difluorobenzonitrile (**2I**).

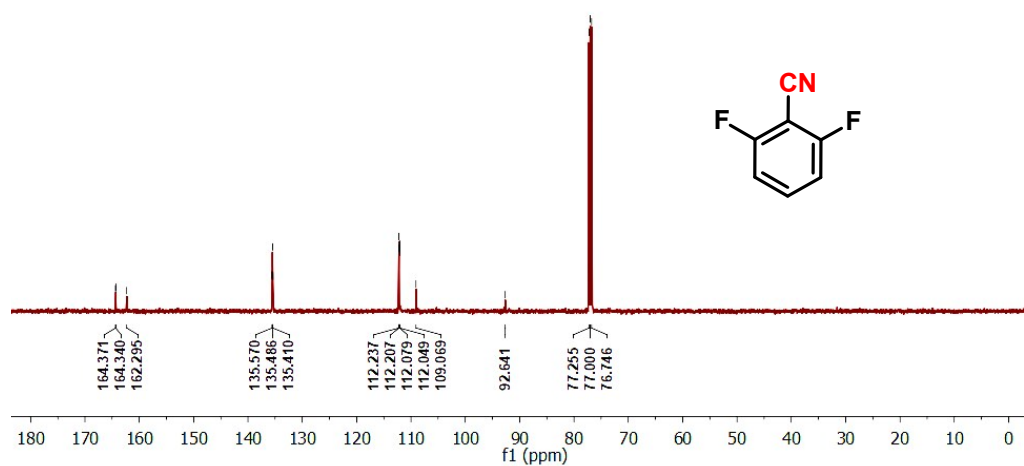


Fig. S30 ¹³C NMR (in CDCl₃) spectrum of 2,6-difluorobenzonitrile (**2I**).

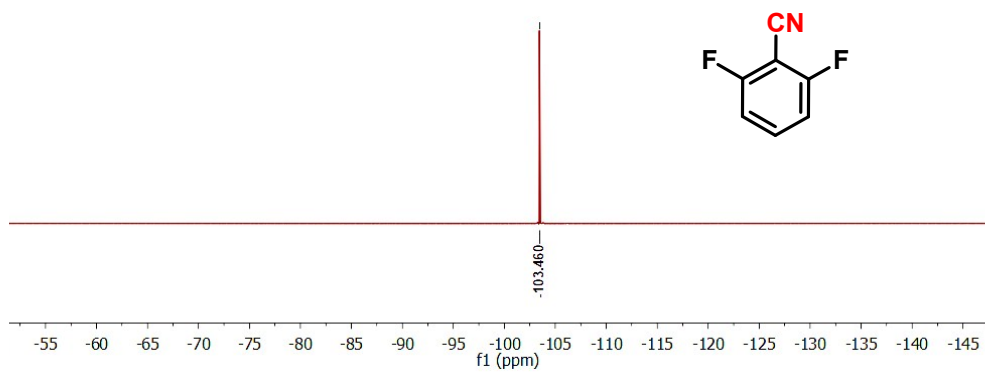


Fig. S31 ¹⁹F NMR (in CDCl₃) spectrum of 2,6-difluorobenzonitrile (**2I**).

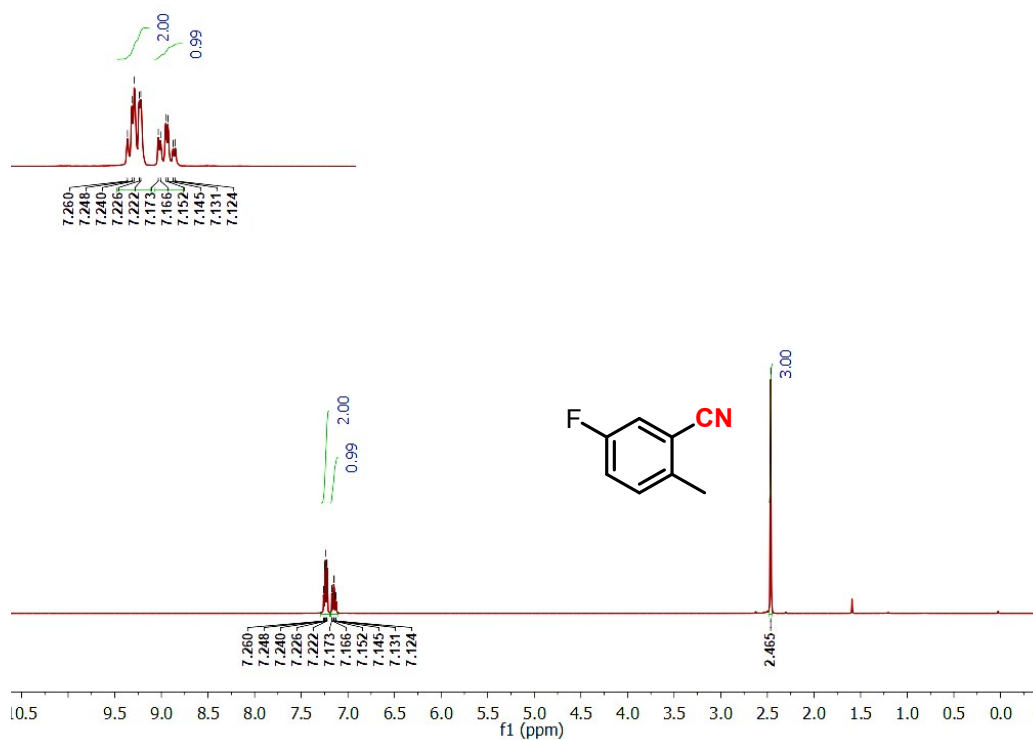


Fig. S32 ¹H NMR (in CDCl₃) spectrum of 5-fluoro-2-methylbenzonitrile (**2m**).³

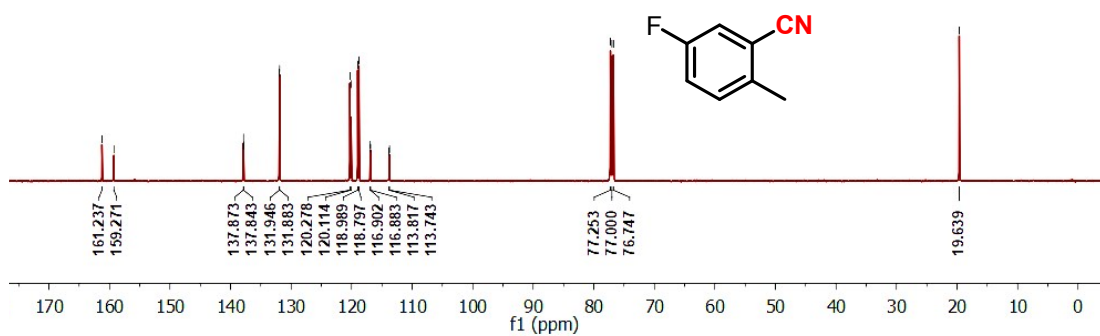


Fig. S33 ¹³C NMR (in CDCl₃) spectrum of 5-fluoro-2-methylbenzonitrile (**2m**).³

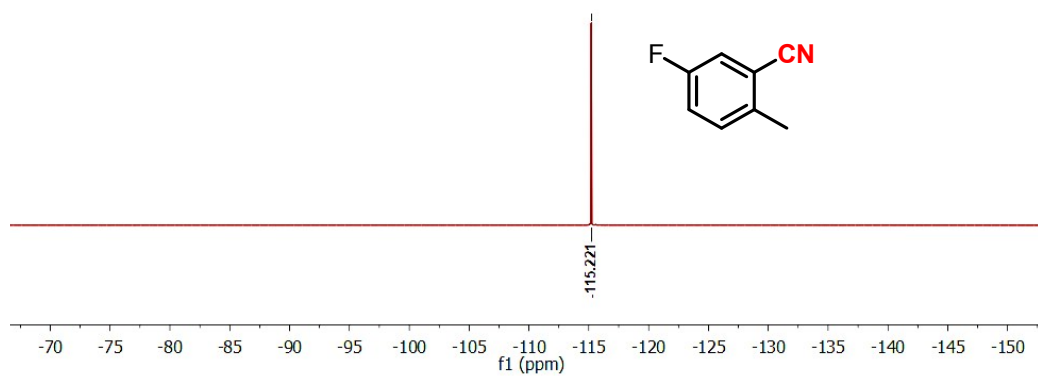


Fig. S34 ¹⁹F NMR (in CDCl₃) spectrum of 5-fluoro-2-methylbenzonitrile (**2m**).

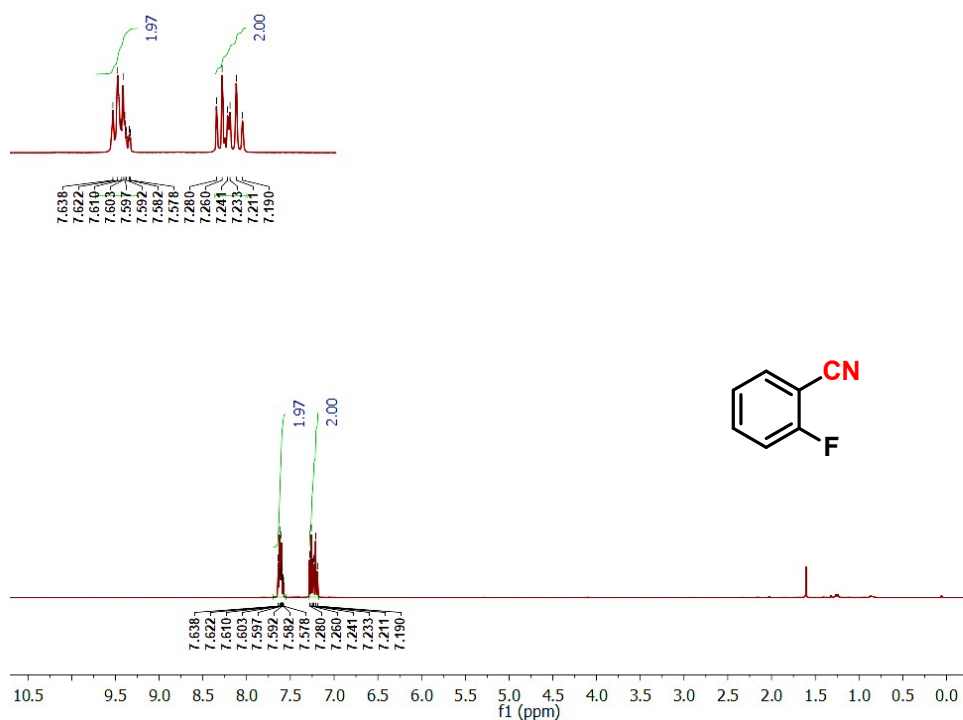


Fig. S35 ¹H NMR (in CDCl₃) spectrum of 2-fluorobenzonitrile (**2n**).⁹

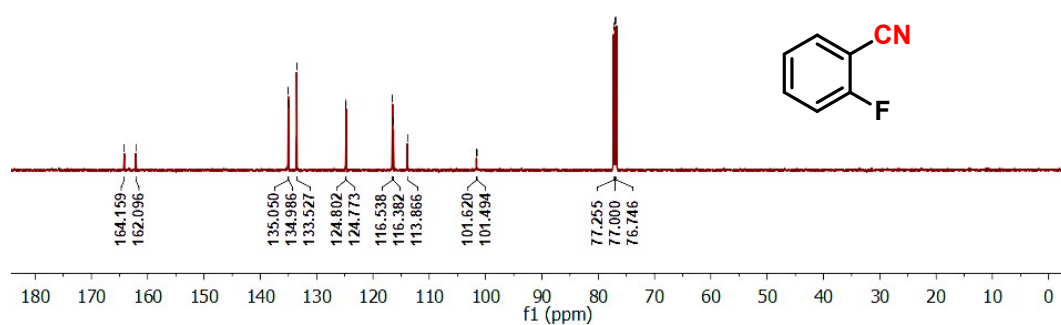


Fig. S36 ¹³C NMR (in CDCl₃) spectrum of 2-fluorobenzonitrile (**2n**).⁹

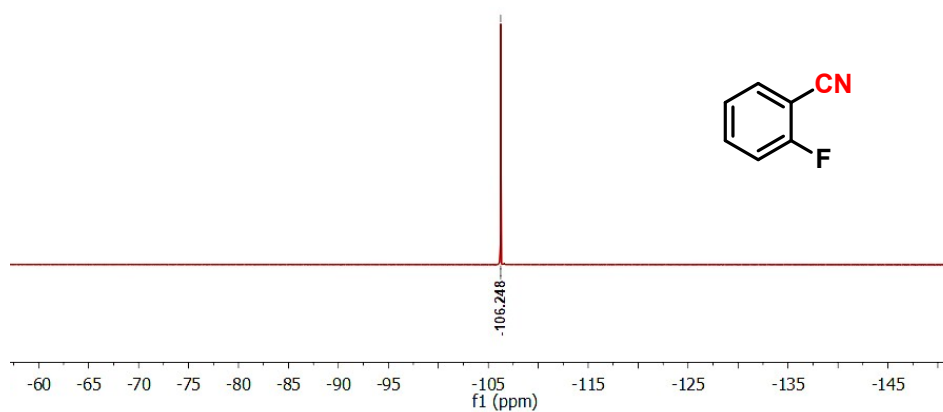


Fig. S37 ¹⁹F NMR (in CDCl₃) spectrum of 2-fluorobenzonitrile (**2n**).⁹

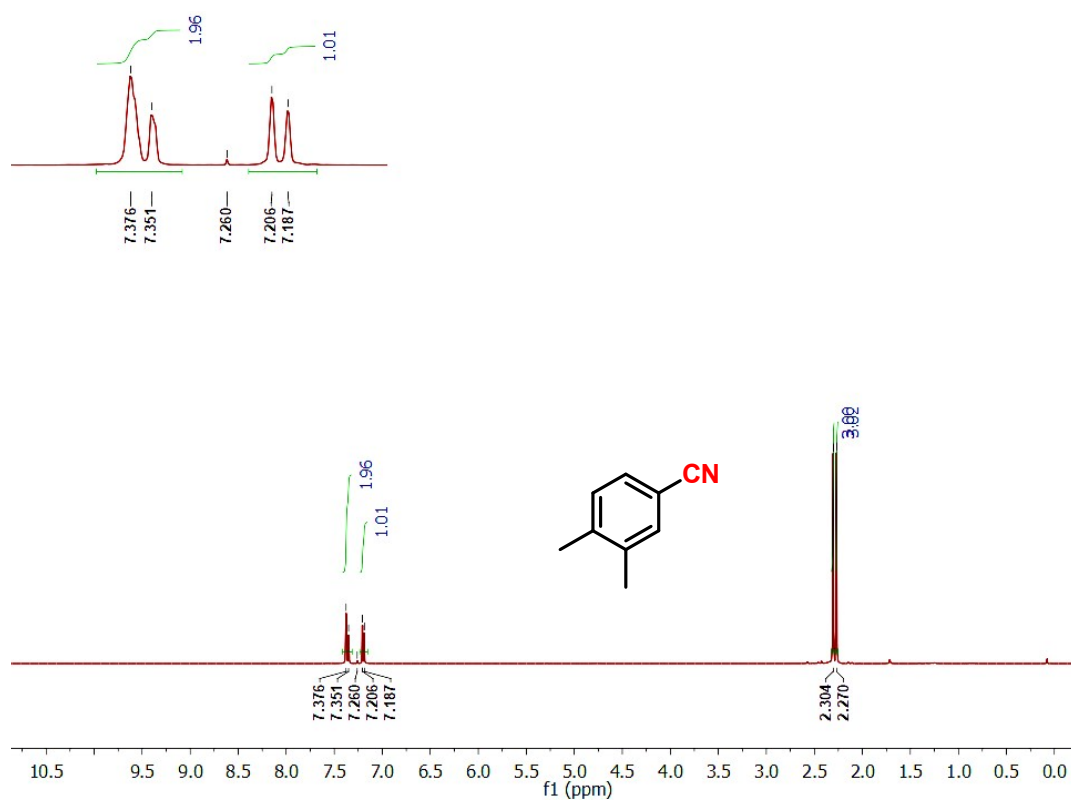


Fig. S38 ¹H NMR (in CDCl₃) spectrum of 3,4-dimethylbenzonitrile (**2o**).¹⁰

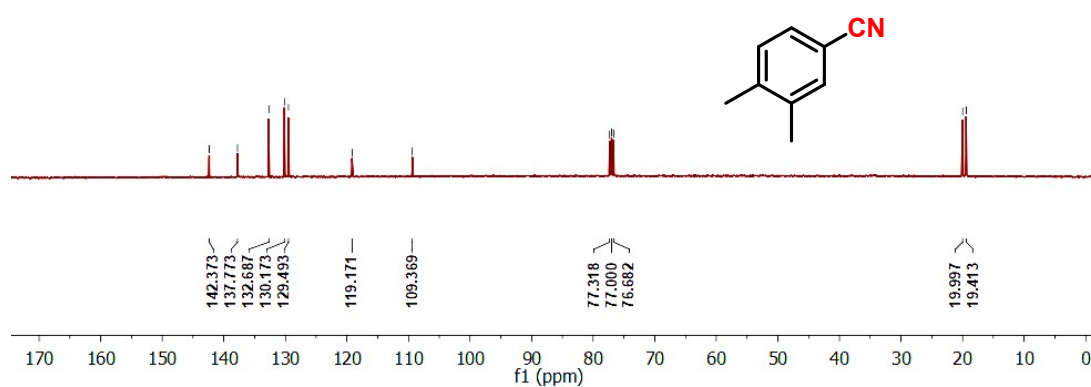


Fig. S39 ¹³C NMR (in CDCl₃) spectrum of 3,4-dimethylbenzonitrile (**2o**).¹⁰

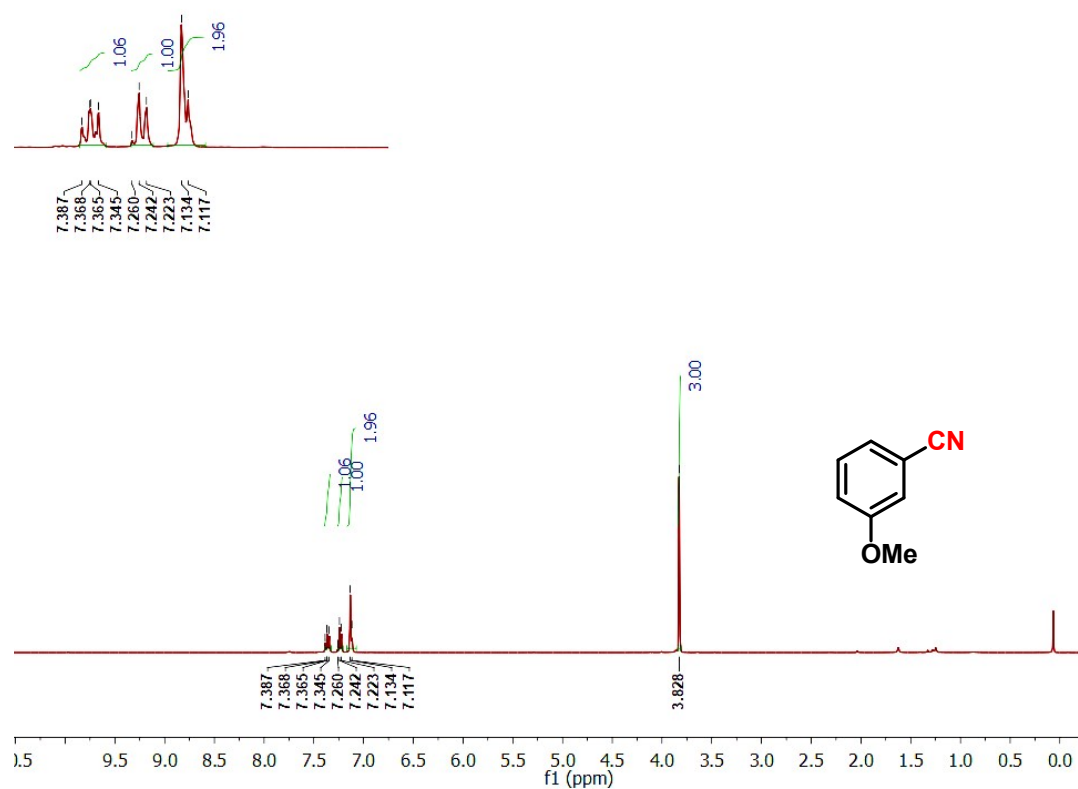


Fig. S40 ¹H NMR (in CDCl₃) spectrum of 3-methoxybenzonitrile (**2p**).³

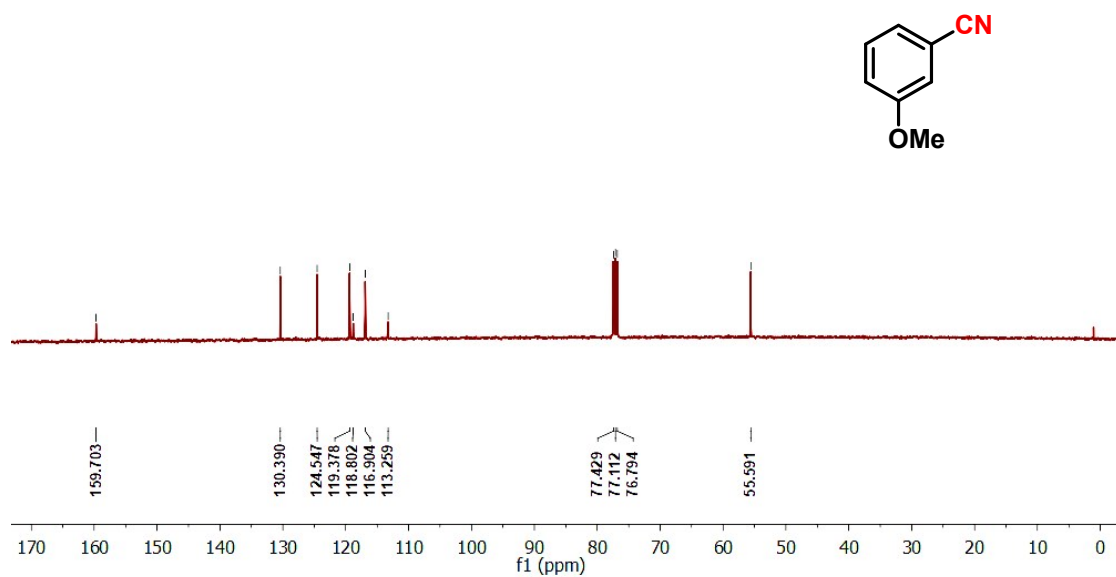


Fig. S41 ¹³C NMR (in CDCl₃) spectrum of 3-methoxybenzonitrile (**2p**).³

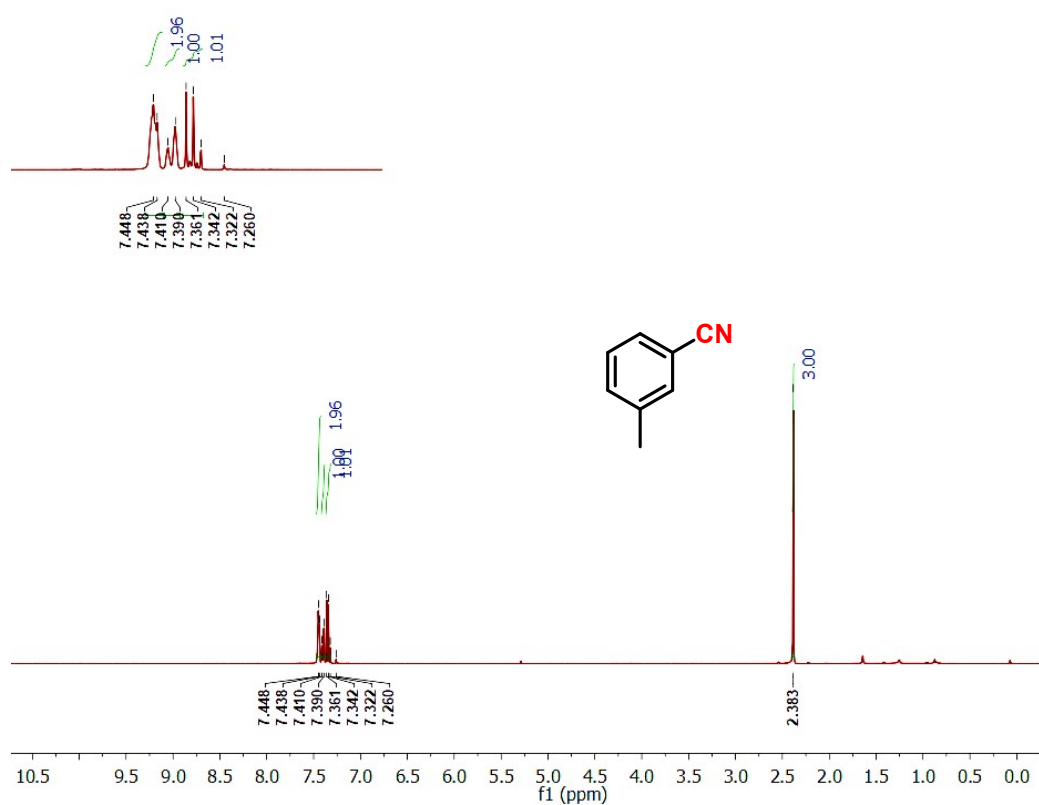


Fig. S42 ¹H NMR (in CDCl₃) spectrum of 3-methylbenzonitrile (**2q**).¹¹

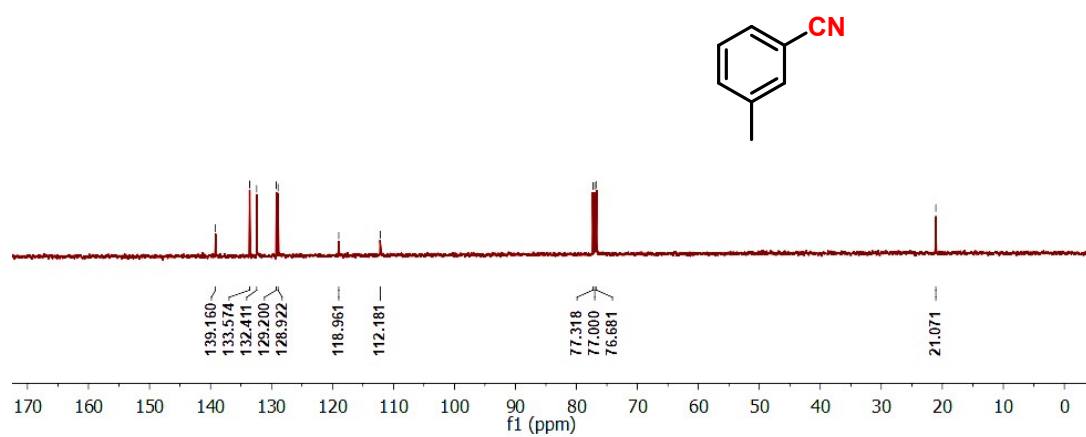


Fig. S43 ¹³C NMR (in CDCl₃) spectrum of 3-methylbenzonitrile (**2q**).¹¹

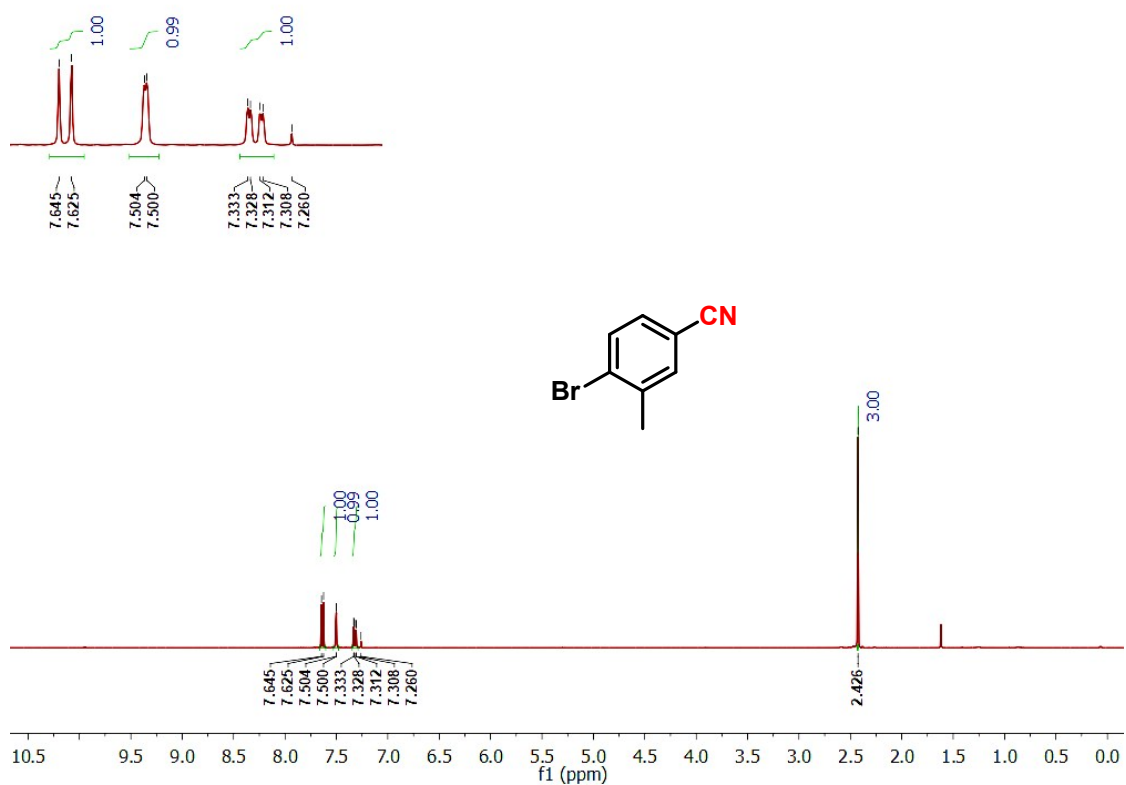


Fig. S45 ¹H NMR (in CDCl₃) spectrum of 4-bromo-3-methylbenzonitrile (**2r**).¹²

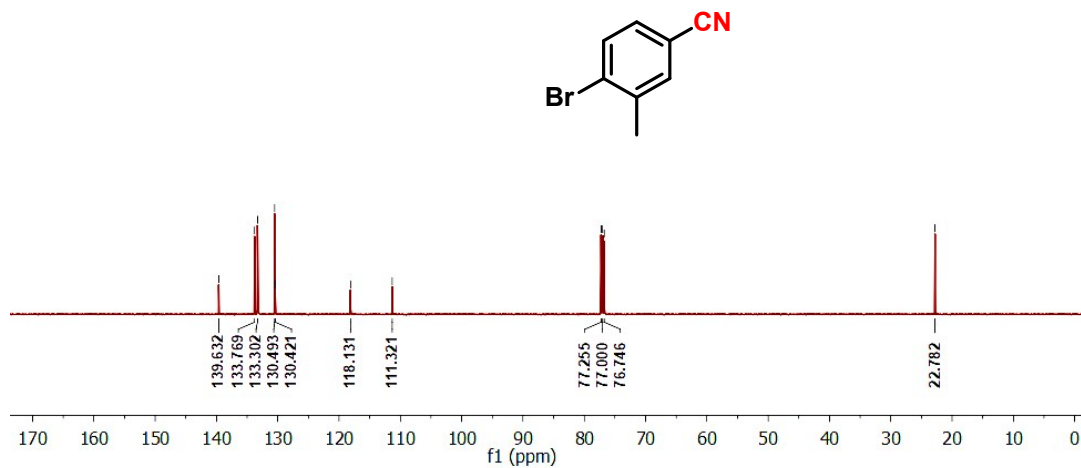


Fig. S45 ¹³C NMR (in CDCl₃) spectrum of 4-bromo-3-methylbenzonitrile (**2r**).¹²

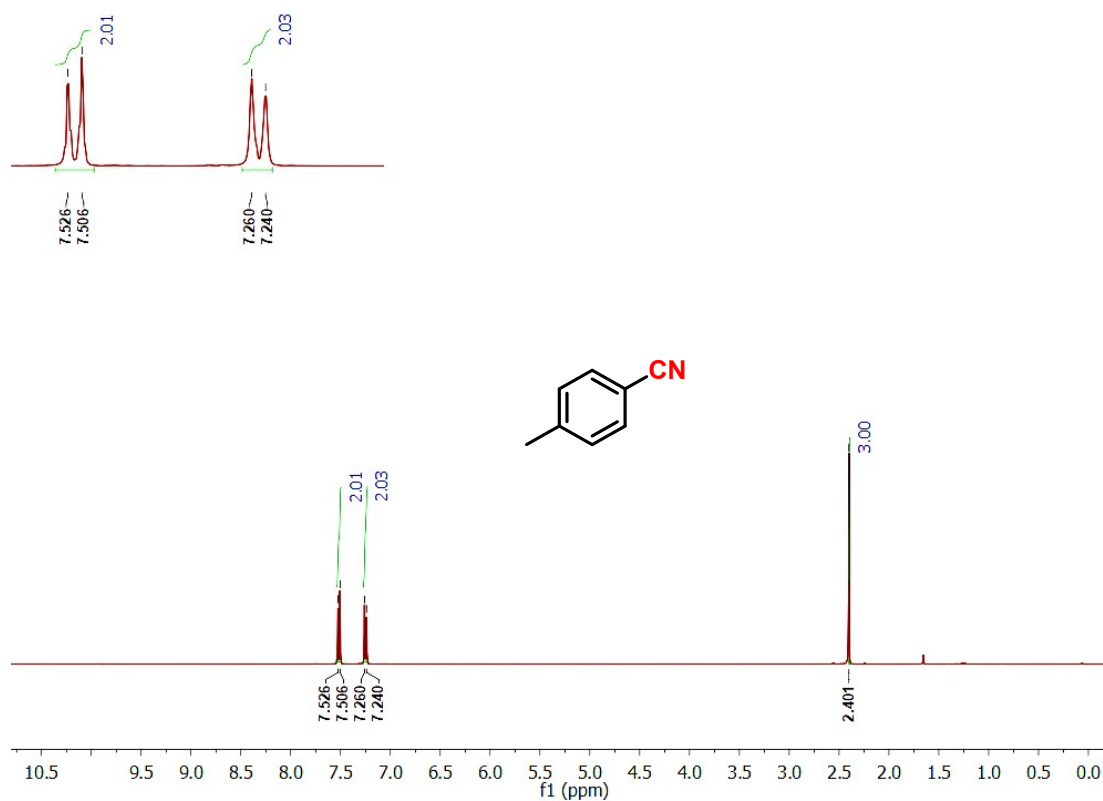


Fig. S46 ¹H NMR (in CDCl₃) spectrum of 4-methylbenzonitrile (2s).¹¹

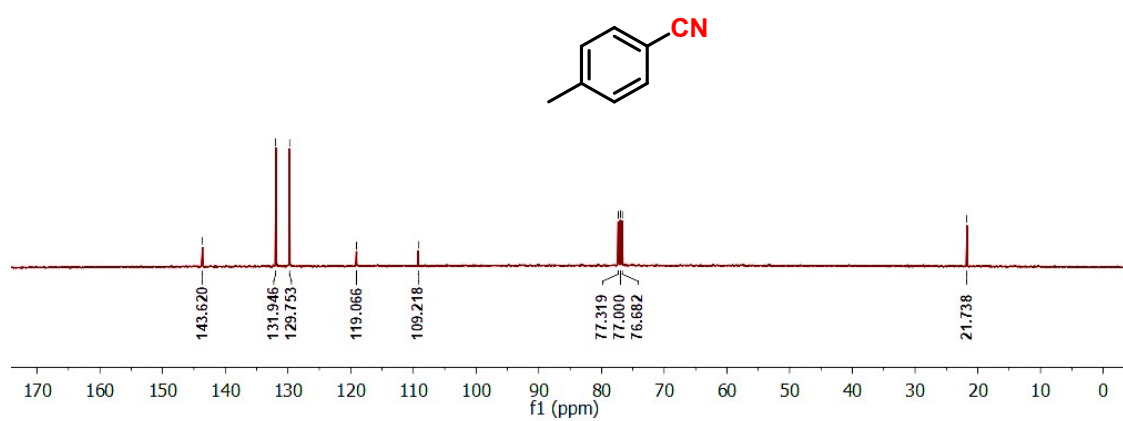


Fig. S47 ¹³C NMR (in CDCl₃) spectrum of 4-methylbenzonitrile (2s).¹¹

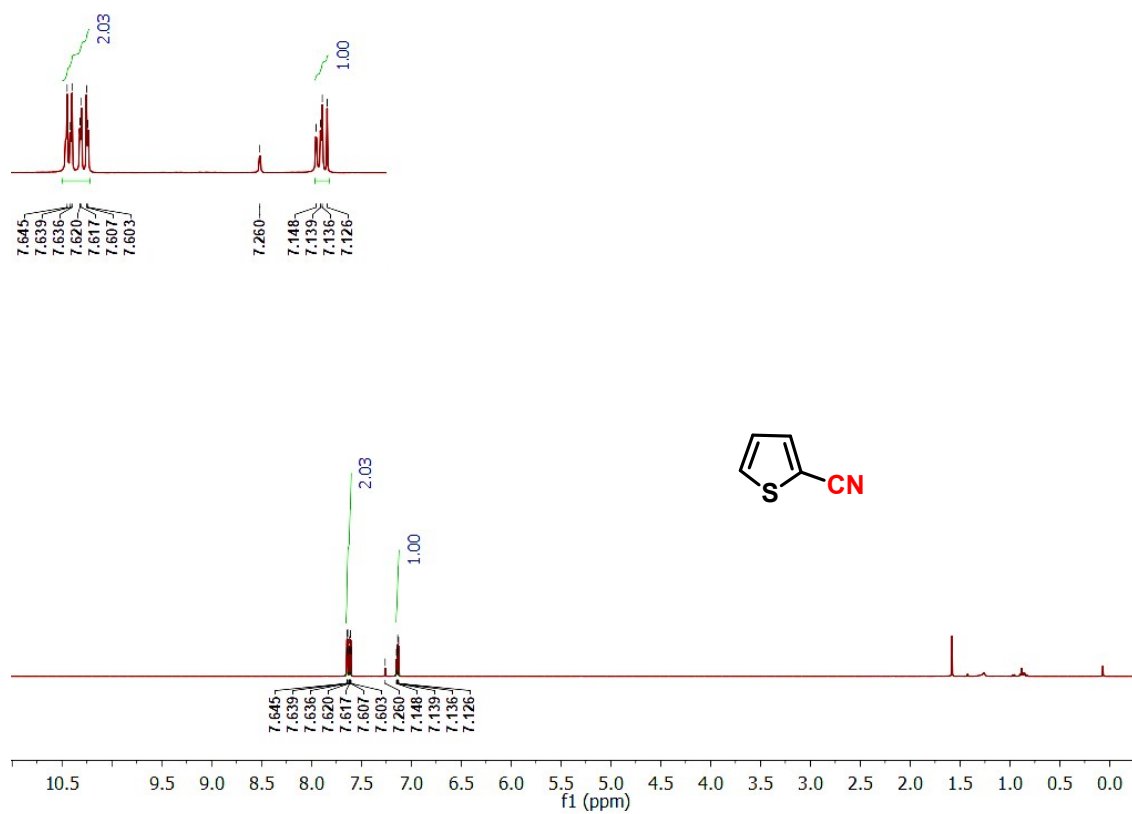


Fig. S48 ¹H NMR (in CDCl₃) spectrum of thiophene-2-carbonitrile (**2t**).⁶

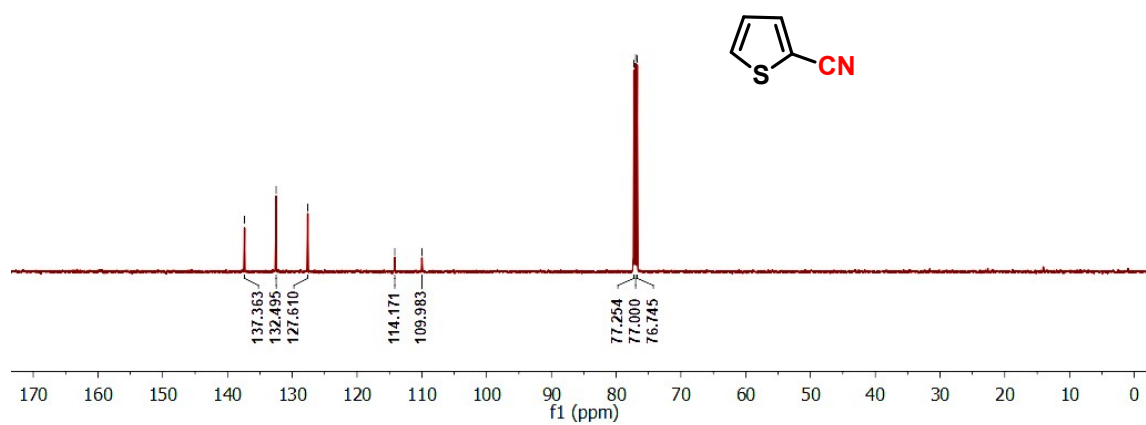


Fig. S49 ¹³C NMR (in CDCl₃) spectrum of thiophene-2-carbonitrile (**2t**).⁶

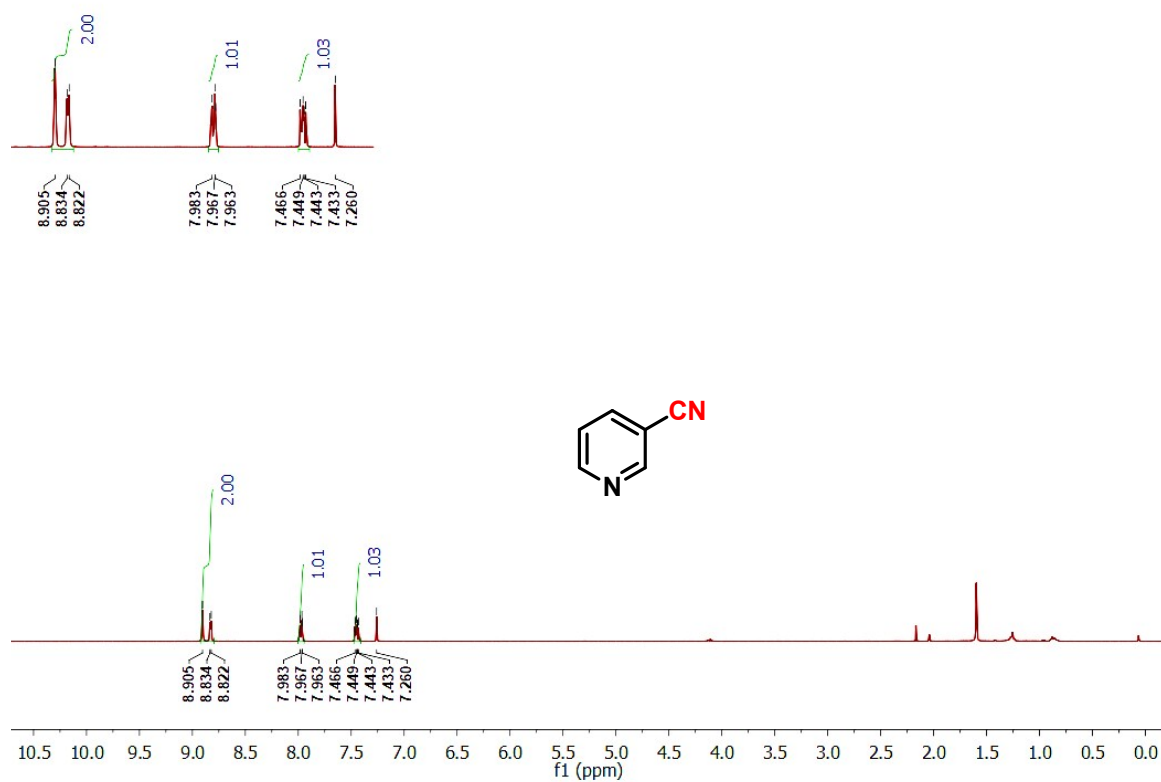


Fig. S50 ¹H NMR (in CDCl₃) spectrum of nicotinonitrile (**2u**).⁶

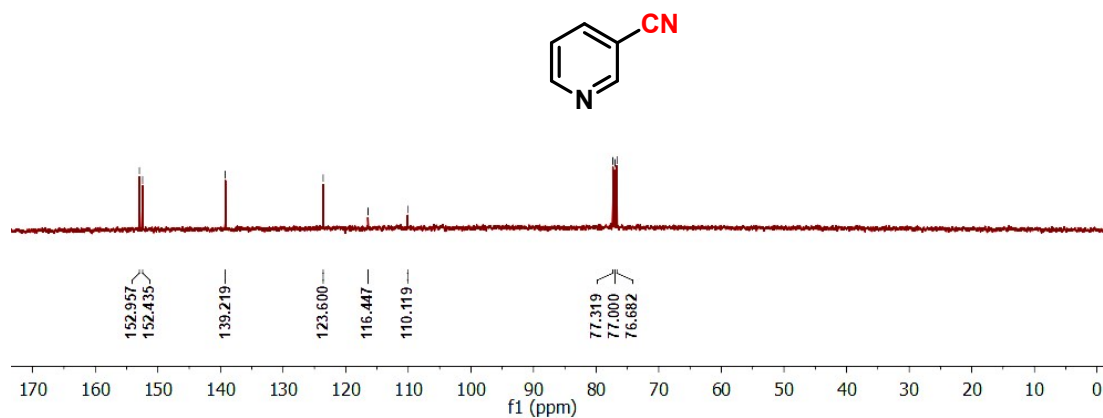


Fig. S51 ¹³C NMR (in CDCl₃) spectrum of nicotinonitrile (**2u**).⁶

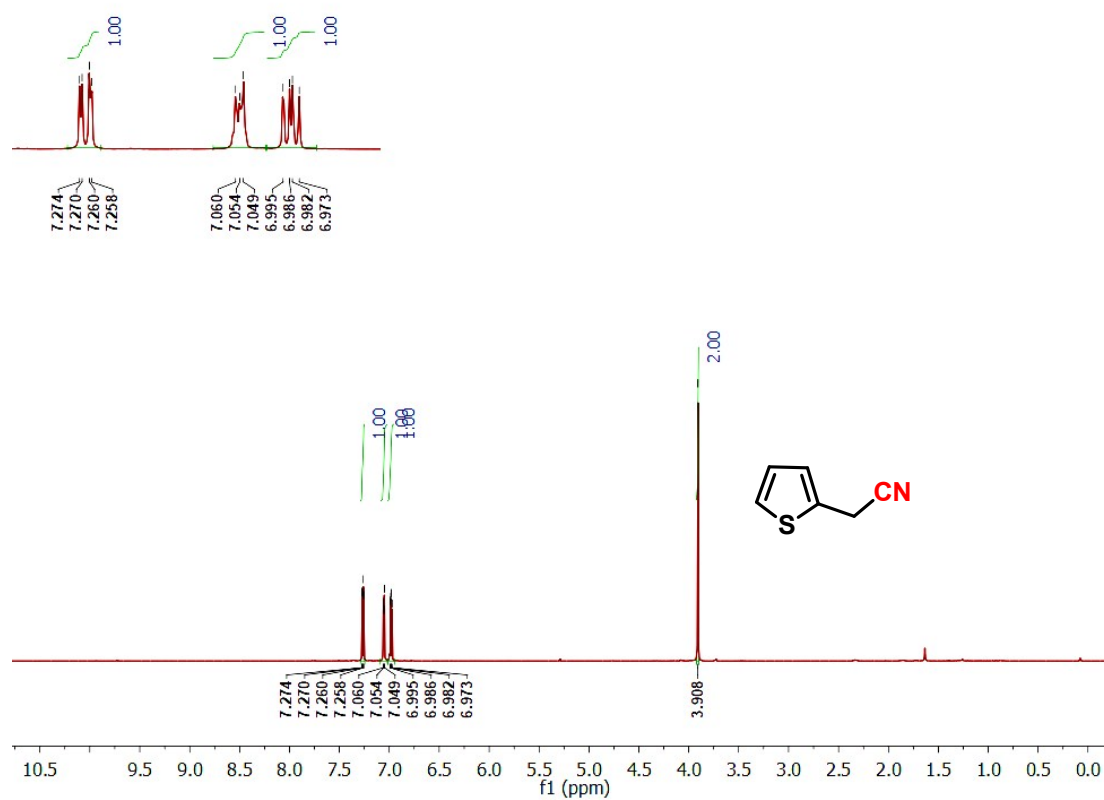


Fig. S52 ¹H NMR (in CDCl₃) spectrum of 2-(thiophen-2-yl)acetonitrile (**2v**).¹³

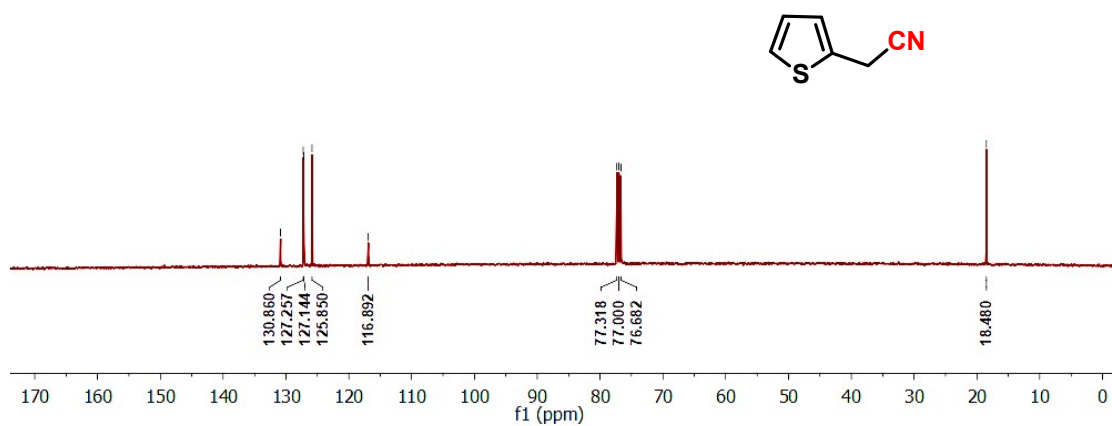


Fig. S53 ¹³C NMR (in CDCl₃) spectrum of 2-(thiophen-2-yl)acetonitrile (**2v**).¹³

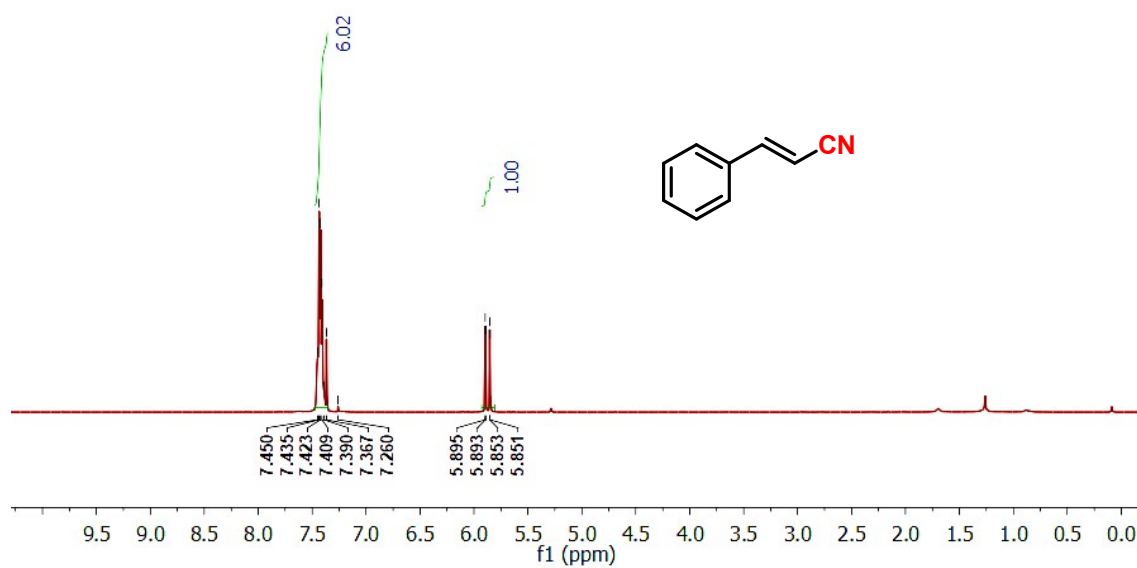


Fig. S54 ¹H NMR (in CDCl₃) spectrum of cinnamitrile (**2aa**).

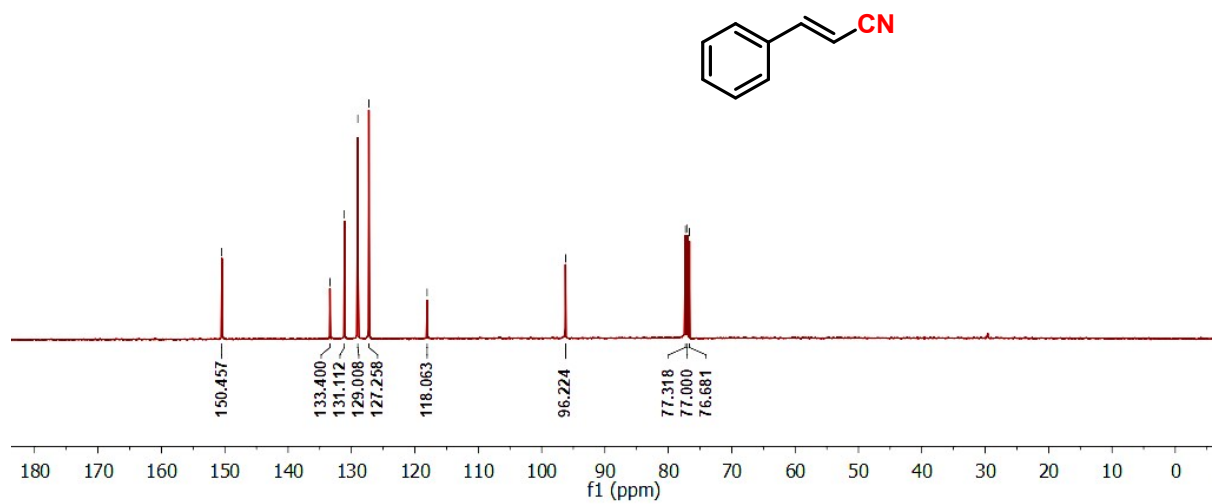


Fig. S55 ¹³C NMR (in CDCl₃) spectrum of cinnamitrile (**2aa**).¹¹

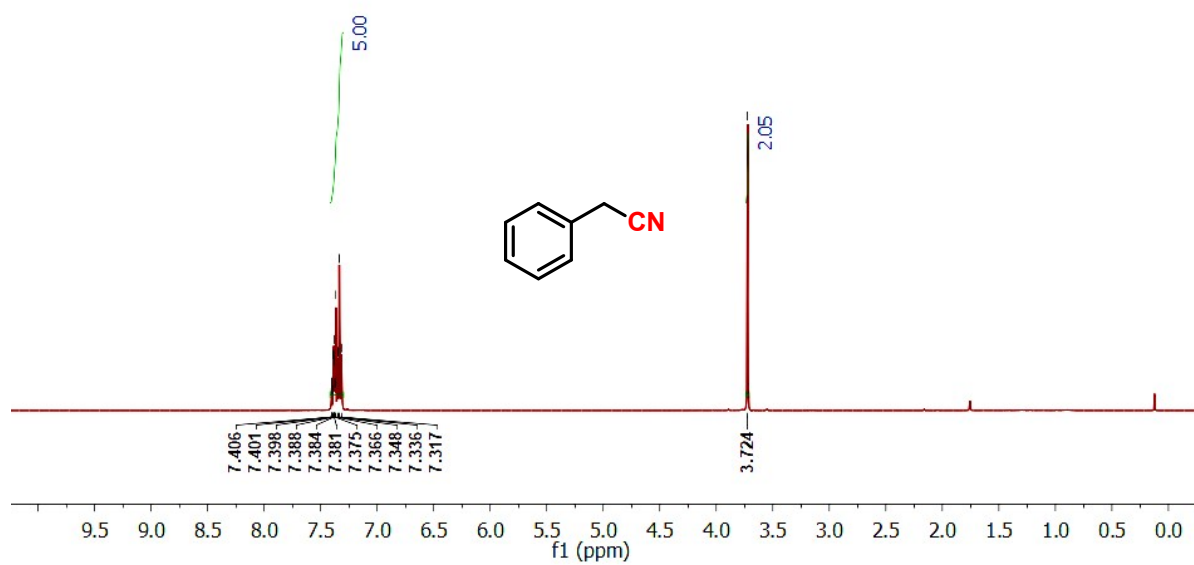


Fig. S56 ¹H NMR (in CDCl₃) spectrum of 2-phenylacetonitrile (**2ab**).⁶

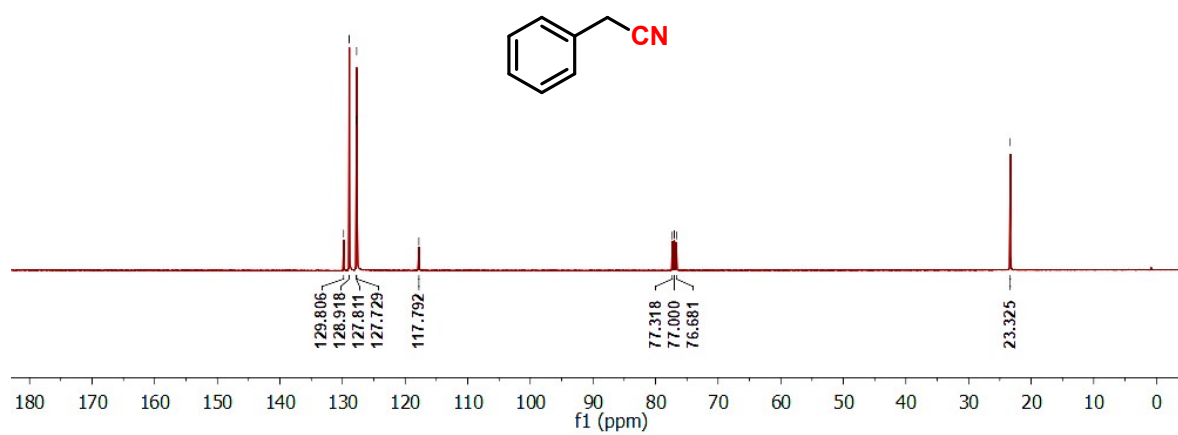


Fig. S57 ¹³C NMR (in CDCl₃) spectrum of 2-phenylacetonitrile (**2ab**).⁶

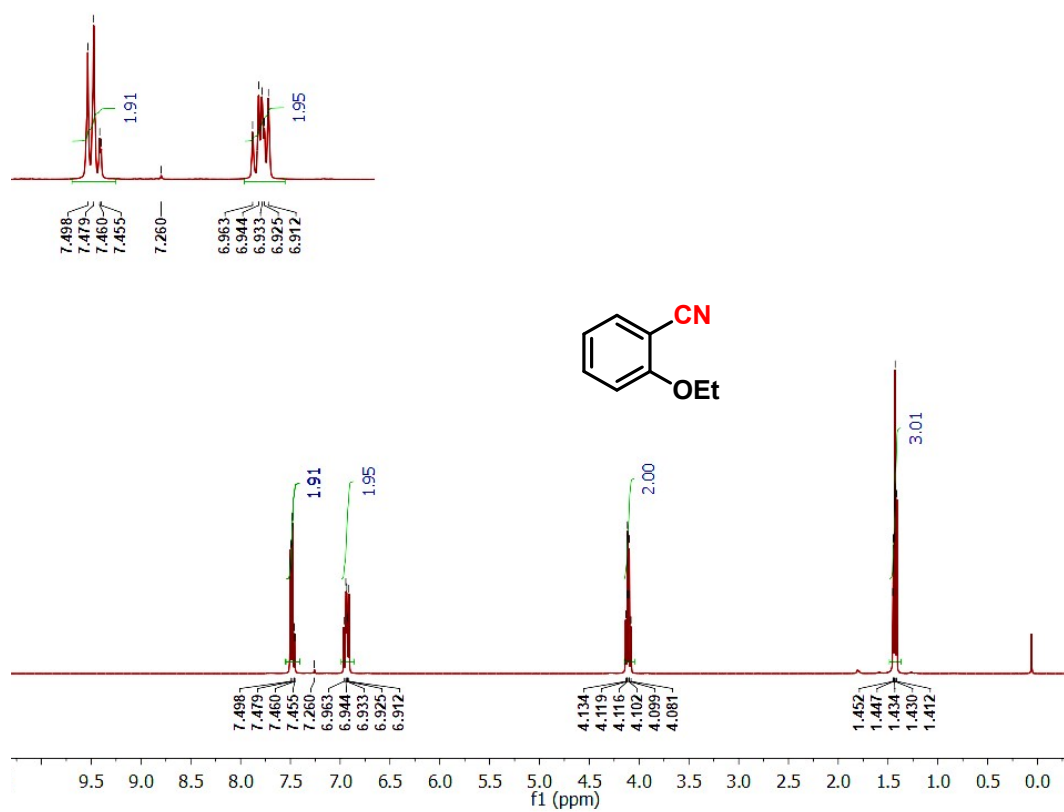


Fig. S58 ¹H NMR (in CDCl₃) spectrum of 2-ethoxybenzonitrile (**2ac**).

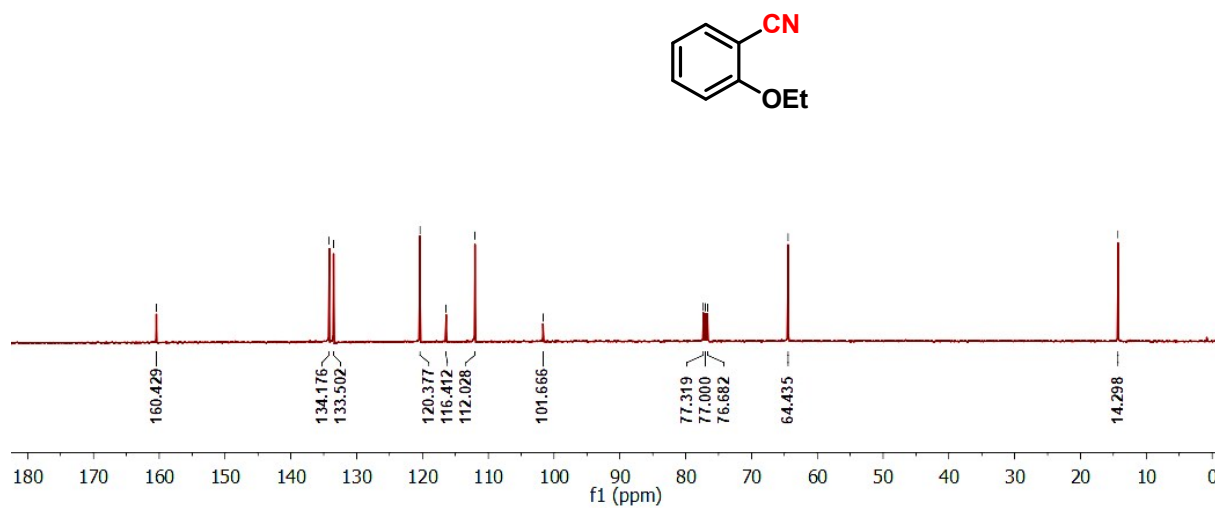


Fig. S59 ¹³C NMR (in CDCl₃) spectrum of 2-ethoxybenzonitrile (**2ac**).

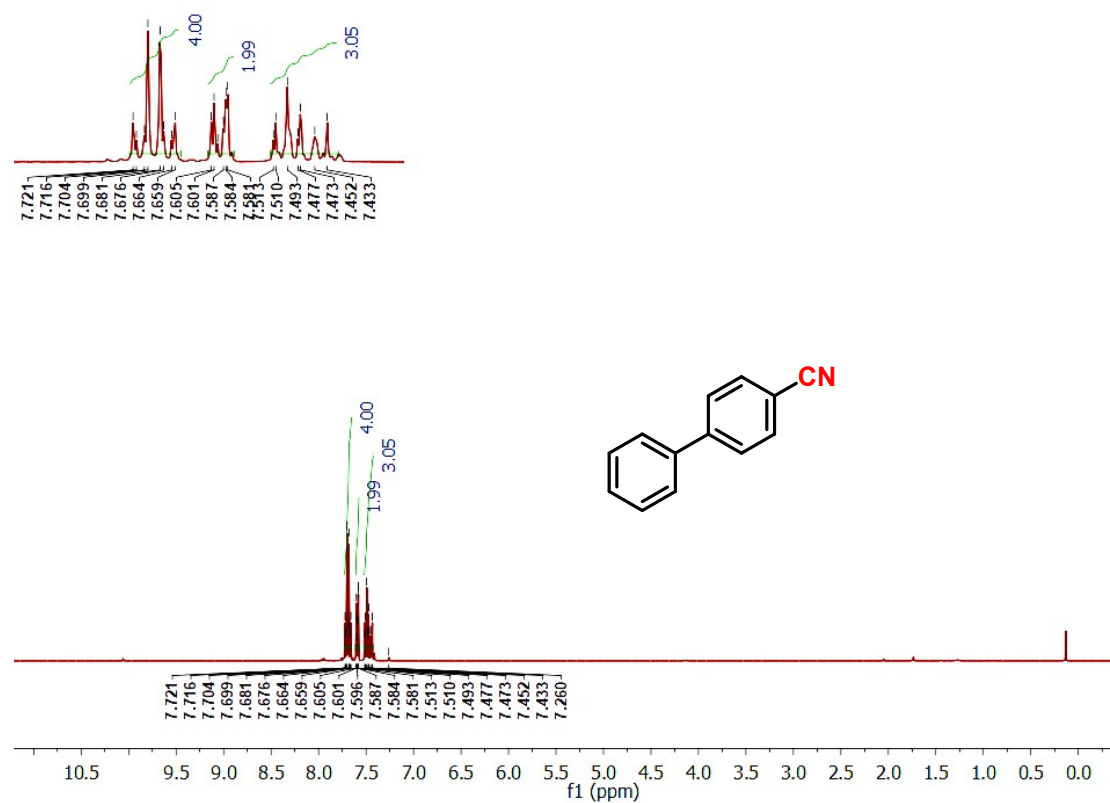


Fig. S60 ¹H NMR (in CDCl₃) spectrum of [1,1'-biphenyl]-4-carbonitrile (**2ad**).¹⁴

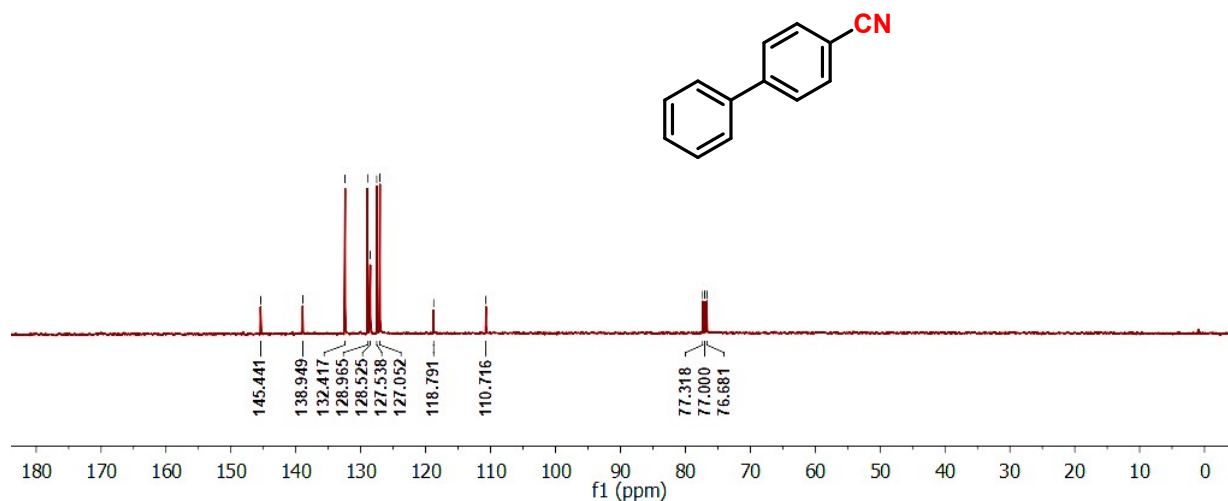


Fig. S61 ¹³C NMR (in CDCl₃) spectrum of [1,1'-biphenyl]-4-carbonitrile (**2ad**).¹⁴

4) Mechanistic Study:

At first we have studied the dehydrogenation process. During the dehydration of primary amides using silane, dehydrogenation is expected to be the first step.⁴ Accordingly, we have performed a stoichiometric reaction using 4-methoxybenzamide, *a*NHC and phenylsilane in a screw cap NMR tube in acetonitrile- d_3 . The reaction was monitored by 1H NMR spectroscopy. During the course of this experiment, a gas was evolved; upon 1H NMR spectroscopic analysis, it was identified as dihydrogen ($\delta = 4.58$ ppm¹ in acetonitrile- d_3). Further help from DFT establishes that such dehydrogenation step occurs through activation of the silane by formation of an *a*NHC-silane adduct. *a*NHC by virtue of its strong Lewis basicity can easily form *a*NHC-silane adduct **Int1**¹⁵ (^{29}Si NMR signal appeared at $\delta = -39.86$ ppm while the ^{29}Si NMR of free DMMS in acetonitrile- d_3 displays a peak at $\delta = -13.00$ ppm). Bertrand and co-workers also reported a comparable ^{29}Si NMR data for CAAC-Silane adduct which appeared at $\delta -36.4$ ppm.¹⁵ The activated *a*NHC-silane adduct undergoes a facile hydride transfer to the amide resulting in an *N*-bound silyl imidate **Int2**, which rapidly equilibrates with *O*-silyl imidate **Int3**.⁴ We were able to locate the *O*-silyl imidate proton during the catalytic reaction of 4-chlorobenzamide with phenylsilane at room temperature (at $\delta = 9.98$ ppm in chloroform- d). However, the DFT study reveals that formation of disilyl imidate from the monosilyl imidate is an uphill process with a free energy barrier of 37.7 kcal/mol which is not achievable at room temperature (see Fig. S62).⁴ A reaction between the *a*NHC and a model imine (benzophenone imine) in acetonitrile- d_3 indeed revealed an interaction between imine and *a*NHC as the imine peak at $\delta = 9.93$ ppm disappeared and such observation has been noted in case of hydrogen bonding reported previously.¹⁶ Furthermore, the catalytic reaction under optimized conditions resulted in the formation of siloxane as a byproduct which was characterized by ^{29}Si NMR spectroscopy (see, Fig. S5).

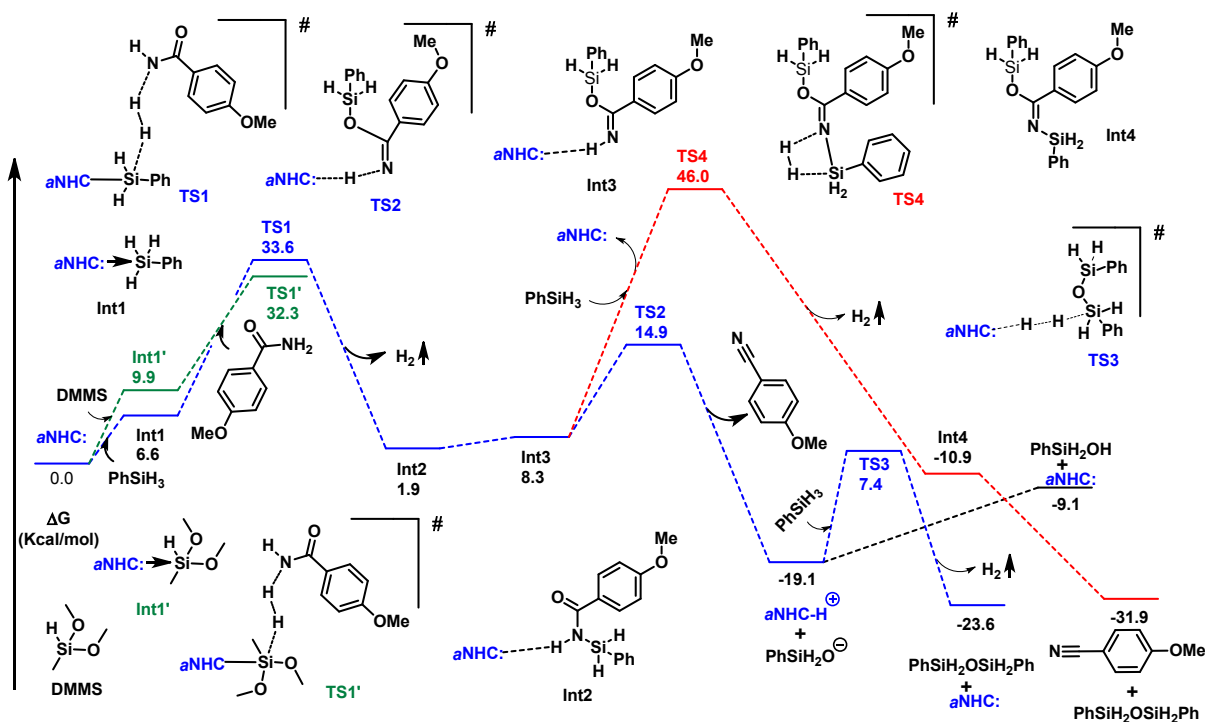


Fig. S62 Computed Gibbs free energy profile for catalytic dehydration of primary amides to nitriles using *a*NHC. Theoretical calculation was carried out with the help of Gaussian16¹⁷ at M062X level of theory by using 6-311+g(2d,p) considering SMD solvent model.^{18-19, 4}

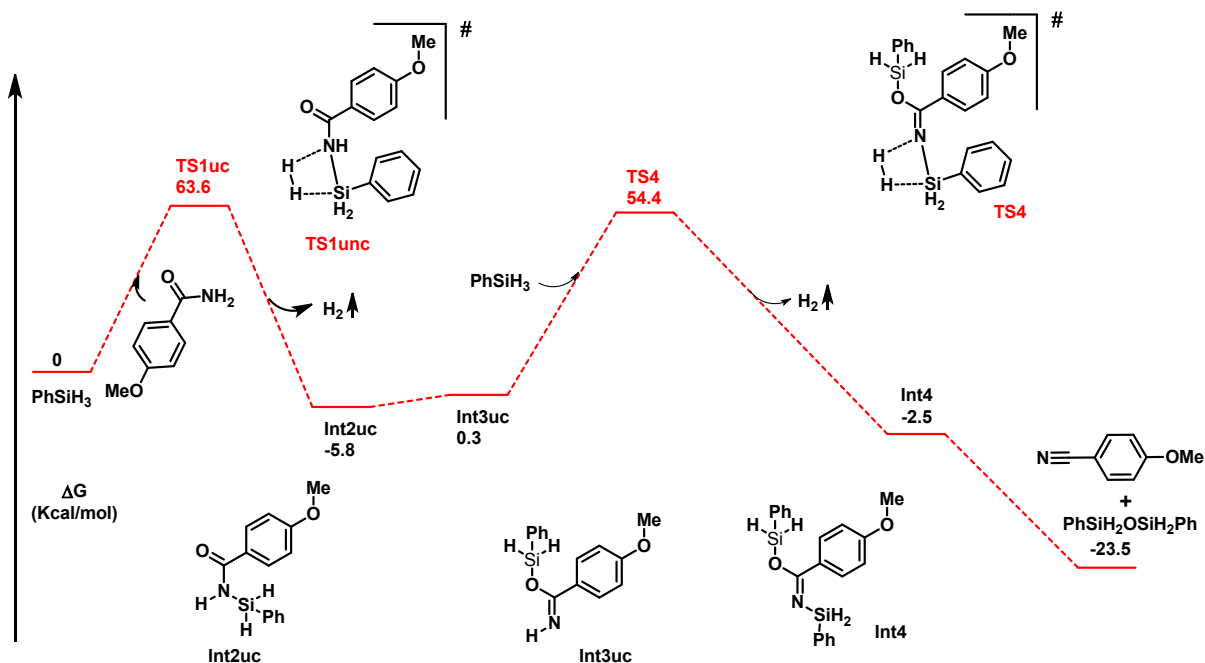


Fig. S63 Computed Gibbs free energy profile for uncatalyzed pathway from primary amide to nitrile.

Table S1 Energies, enthalpies, and free energies (in Hartree) of the structures calculated with M06-2X/6-311+G(2d,p)-SMD(Acetonitrile)//B3LYP/6-31G(d).

Structure	ZPE	ΔE	ΔH	ΔG	E	H	G	IF (cm ⁻¹)	Infrared
AmideOMe	0.160481	0.170146	0.171090	0.125732	-515.275941	-515.274997	-515.320356		
PhSiH3	0.115718	0.122348	0.123292	0.085067	-522.766416	-522.765471	-522.803696		
<i>a</i> NHC	0.731150	0.769219	0.770163	0.664216	-	-	-		
					1621.155853	1621.154909	1621.260855		
Int1	0.846781	0.893033	0.893977	0.767116	-	-	-		
					2143.928081	2143.927136	2144.053997		
TS1uncat	0.272815	0.289207	0.290152	0.228777	-	-	-	-	7949.1443
					1037.962212	1037.961267	1038.022642	1496.6	
Int3uncat	0.259274	0.275515	0.276459	0.214818	-	-	-		
					1036.893396	1036.892451	1036.954092		
H2	0.010111	0.012471	0.013416	-	-1.155510	-1.154565	-1.169357		
				0.001376					
TS1	1.004060	1.061030	1.061974	0.913216	-	-	-	-	12438.96
					2659.183449	2659.182505	2659.331263	1019.7	
Int2	0.990847	1.047255	1.048199	0.900331	-	-	-		
					2658.065472	2658.064528	2658.212397		
Int3	0.990739	1.047217	1.048161	0.900118	-	-	-		
					2658.055047	2658.054103	2658.202146		
Int2uncat	0.259473	0.275749	0.276693	0.215201	-	-	-		
					1036.903289	1036.902345	1036.963836		
TSt	0.258337	0.274018	0.274962	0.214905	-	-	-	-	21.98
					1036.879700	1036.878755	1036.938812	197.15	
TS2	0.985265	1.041539	1.042483	0.894897	-	-	-	-1401.12	13198.31
					2658.045030	2658.044086	2658.191673		
TS3	0.966081	1.021140	1.022084	0.877184	-	-	-	-	15493.65
					2741.981128	2741.980184	2742.125084	1276.4	
Pdt	0.132444	0.140623	0.141567	0.099524	-438.840499	-438.839554	-438.881598		
PhSiO	0.109654	0.116890	0.117835	0.077660	-597.563096	-597.562152	-597.602326		
<i>a</i> NHC cation	0.744121	0.782589	0.783533	0.676563	-	-	-		
					1621.655875	1621.654931	1621.761901		
TS4	0.370401	0.394023	0.394968	0.316593	-	-	-	-	7702.98
					1559.594182	1559.593238	1559.671612	1400.8	
Int4	0.357326	0.380539	0.381483	0.303655	-	-	-		
					1558.516130	1558.515186	1558.593014		
PhSiOSiPh	0.221562	0.236156	0.237100	0.177898	-	-	-		
					1119.686602	1119.685658	1119.744861		
DMMS	0.131172	0.140340	0.141284	0.097459	-560.177663	-560.176719	-560.220545		
<i>a</i> NHC-DMMS	0.862061	0.909960	0.910904	0.782473	-	-	-		
					2181.338005	2181.337061	2181.465493		
TS1'	1.020198	1.079253	1.080197	0.929438	-	-	-	-	9212.89
					2696.600292	2696.599348	2696.750106	962.57	
DMMSO	0.124975	0.134792	0.135736	0.089848	-634.980202	-634.979257	-635.025145		
DMMS2O	0.251316	0.271292	0.272236	0.202825	-	-	-		
					1194.534400	1194.533456	1194.602866		
DMMSOH	0.136431	0.146575	0.147520	0.101092	-635.465291	-635.464347	-635.510774		

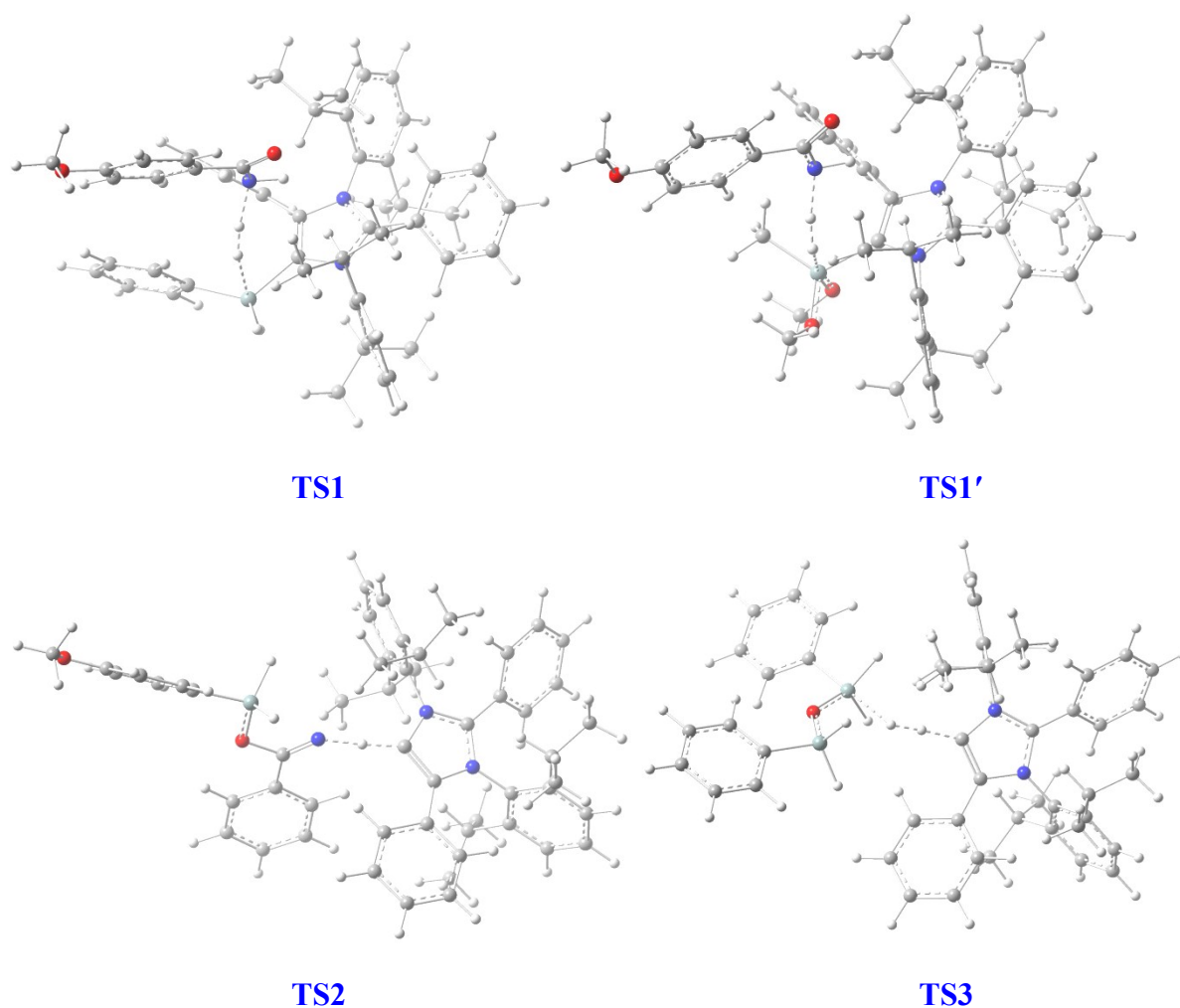


Fig. S64 Optimized structures of the transition states involved in the potential energy surface of catalytic dehydration of primary amides by the *a*NHC catalyst. **TS1'** when DMMS was used.

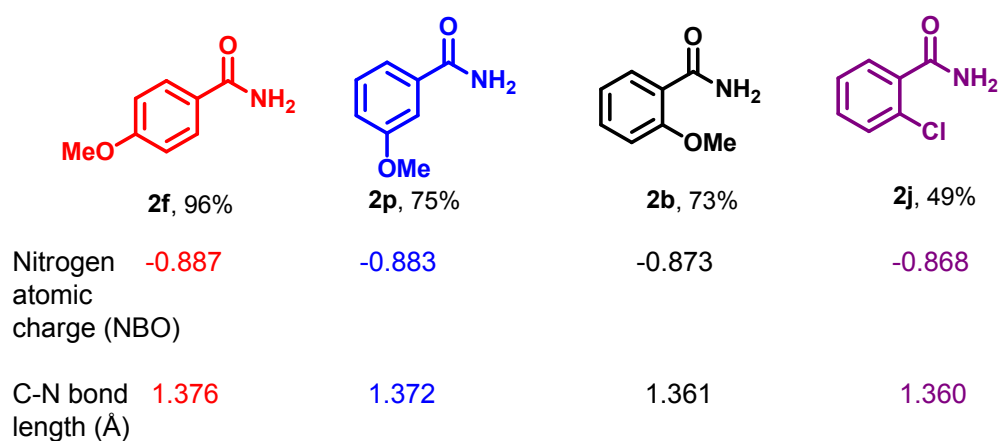


Fig. S65 The calculated atomic charge on amide nitrogen and the C-N bond length using B3LYP/6-31+G(d,p).

AmideOMe

0 1

C	1.10658000	-0.98959700	0.07716500
C	-0.27982300	-1.12382700	0.06730000
C	-1.11926000	-0.00894900	-0.02350500
C	-0.53227900	1.26383700	-0.13028300
C	0.84683000	1.41400000	-0.12780500
C	1.67758400	0.28733400	-0.01780800
H	1.72774700	-1.87437800	0.15563200
H	-0.73787200	-2.10555700	0.13002700
H	-1.15316700	2.14709100	-0.25270000
H	1.30914500	2.39161400	-0.22042000
C	-2.59638500	-0.24921100	-0.01935200
N	-3.39673500	0.85334300	0.20291200
H	-4.37539400	0.63835200	0.34424800
H	-3.03739000	1.63350500	0.73451900
O	-3.08025400	-1.35591200	-0.22795800
O	3.01494300	0.53995200	-0.01911800
C	3.91112100	-0.55858500	0.07143700
H	4.91340800	-0.12759400	0.04866400
H	3.77523400	-1.11272100	1.00912300
H	3.79170900	-1.24604200	-0.77575200

aNHC

0 1

C	0.41060500	-1.92083600	-0.06179900
C	0.47402000	0.39532900	-0.01568200
C	-0.87890900	-1.39935600	-0.13120900
N	1.19543000	-0.76381900	-0.00697600
N	-0.82978700	0.01749600	-0.08135500
C	-2.09794400	-2.21754200	-0.25390800
C	-3.33866000	-1.77859100	-0.75403900
C	-1.98799600	-3.57459100	0.12014600
C	-4.42138700	-2.65516800	-0.85954100
H	-3.47321100	-0.75265300	-1.07055700
C	-3.06688200	-4.44378900	0.00747400
H	-1.02814300	-3.92149000	0.48687700
C	-4.29678700	-3.99001900	-0.47905300
H	-5.36606700	-2.28480200	-1.25025700
H	-2.94885500	-5.48260200	0.30604300
H	-5.14175300	-4.66833300	-0.56300300
C	1.00466200	1.76856800	-0.00164600
C	2.10758300	2.10339100	-0.81115900
C	0.44731400	2.77486600	0.80957800
C	2.63353100	3.39310900	-0.80372300
H	2.54991000	1.35248700	-1.45401600
C	0.97369400	4.06507900	0.80898900

H	-0.40157300	2.54988700	1.44180600
C	2.06997600	4.38138400	0.00524600
H	3.48330700	3.62580100	-1.43950400
H	0.52607300	4.82312700	1.44588300
H	2.48061900	5.38724800	0.00889900
C	2.63299700	-0.85210800	0.13180000
C	3.40240400	-1.16791200	-1.00598300
C	3.20416200	-0.69339700	1.41037000
C	4.78764700	-1.28620800	-0.83874400
C	4.59466000	-0.81562600	1.51852200
C	5.38103500	-1.10286500	0.40652700
H	5.40996200	-1.52875100	-1.69464000
H	5.06839500	-0.69581700	2.48752700
H	6.45879000	-1.19562400	0.51352700
C	-1.94536200	0.93772500	-0.04850900
C	-2.28361900	1.64907500	-1.21980600
C	-2.67625600	1.07016900	1.15359700
C	-3.37748200	2.52105300	-1.15505000
C	-3.76002100	1.95676100	1.15603500
C	-4.10914900	2.67783600	0.01812300
H	-3.66181800	3.08179800	-2.04085400
H	-4.34127300	2.08037500	2.06537600
H	-4.95520400	3.35945000	0.04442800
C	-2.34671500	0.29044800	2.42750800
H	-1.48559200	-0.35199300	2.22318800
C	-1.53559500	1.48453100	-2.54146300
H	-0.68626700	0.81656900	-2.37234300
C	2.76355900	-1.43307100	-2.36715400
H	1.77201500	-0.96707500	-2.36867200
C	2.34098900	-0.50010100	2.65430400
H	1.41777000	0.00393800	2.35106900
C	-2.42653500	0.82059100	-3.61123800
H	-3.30459500	1.43661000	-3.83900800
H	-1.86247600	0.68704100	-4.54175600
H	-2.77855400	-0.16363600	-3.28622300
C	-0.97399700	2.82487300	-3.05457900
H	-0.32884400	3.30194300	-2.31087900
H	-0.38379000	2.66104700	-3.96377500
H	-1.77720900	3.52714200	-3.30716100
C	-3.51346200	-0.62962900	2.84183400
H	-3.22560700	-1.22997600	3.71261700
H	-4.40118300	-0.04812000	3.11882600
H	-3.79116700	-1.31133300	2.03382200
C	-1.96503300	1.22170500	3.59613900
H	-1.72527400	0.62680000	4.48504900
H	-1.09009300	1.83829600	3.36396000
H	-2.78851000	1.89512500	3.86119300
C	1.94054100	-1.87825600	3.22383000

H	1.42983900	-2.47640400	2.46205700
H	2.82718000	-2.43076100	3.55820800
H	1.27061500	-1.75917700	4.08463600
C	2.99169800	0.38217700	3.73172200
H	3.86355700	-0.09904600	4.18979200
H	3.31136400	1.34748100	3.32359900
H	2.27290100	0.57451900	4.53651900
C	2.54214200	-2.94744900	-2.56283100
H	3.49732200	-3.48688900	-2.54271200
H	1.89739300	-3.33228700	-1.76705900
H	2.06268100	-3.14129500	-3.53047700
C	3.55410000	-0.82990500	-3.54174300
H	3.74437500	0.24139000	-3.40373800
H	4.52176800	-1.32418800	-3.68504200
H	2.98855900	-0.95509200	-4.47220800

PhSiH₃

0 1

Si	-2.34770000	0.00000300	0.00607800
H	-2.86429100	-1.20910600	-0.69173000
H	-2.86330700	1.21798500	-0.67682200
H	-2.89357600	-0.00855600	1.39291100
C	-0.46849600	0.00000700	-0.01209900
C	0.25667200	-1.20512800	-0.00990700
C	0.25663400	1.20508800	-0.00993300
C	1.65215100	-1.20772300	0.00331200
H	-0.27188300	-2.15607800	-0.02356100
C	1.65218000	1.20769600	0.00332100
H	-0.27195500	2.15600100	-0.02356400
C	2.35227000	0.00001500	0.01076300
H	2.19260800	-2.15080000	0.00348700
H	2.19257800	2.15080500	0.00350000
H	3.43916400	-0.00001500	0.01795400

TS1uncat

0 1

Si	2.31571100	1.69224100	-0.55711800
H	2.90337400	1.84387200	-1.93532100
H	2.86012700	2.76478500	0.31836300
H	1.10357400	2.75428700	-1.24966700
C	3.09452900	0.00385800	-0.15595800
C	3.98522400	-0.55526600	-1.08766400
C	2.89626100	-0.69100200	1.05262800
C	4.65411700	-1.75481200	-0.83028000
H	4.15768600	-0.04558100	-2.03330800
C	3.56453100	-1.88558700	1.31954700

H	2.20685900	-0.29359200	1.79207300
C	4.44523700	-2.42216900	0.37621900
H	5.33443800	-2.16716900	-1.57151200
H	3.39896900	-2.40056500	2.26299500
H	4.96374600	-3.35538600	0.58223300
H	0.30336100	3.11658200	-0.73065200
N	-0.44498700	3.11119400	0.34582800
H	0.34422800	3.48679000	0.88402400
C	-0.37864100	1.76266300	0.39658400
C	-1.58715600	0.95880500	0.23342600
C	-2.85833300	1.56877700	0.26815600
C	-1.50448400	-0.43059300	0.04697700
C	-4.00429800	0.81234100	0.10799500
H	-2.91640600	2.64097200	0.42001000
C	-2.65147100	-1.20062000	-0.10846800
H	-0.52759900	-0.90216100	0.02567600
C	-3.91089800	-0.57921300	-0.08125400
H	-4.99022300	1.26527700	0.12893400
H	-2.56050100	-2.27080000	-0.25213000
O	0.76750000	1.15660600	0.39871400
O	-5.09135600	-1.22993400	-0.22319300
C	-5.07848200	-2.63976900	-0.41589400
H	-6.12481400	-2.93575000	-0.50361800
H	-4.54401500	-2.91303600	-1.33410700
H	-4.62382500	-3.15611700	0.43862400

Int3uncat

0 1

C	-4.14633900	0.52622100	0.09779400
C	-2.97818100	1.28542300	0.09818400
C	-1.71641100	0.69065300	-0.02014500
C	-1.65314000	-0.71045200	-0.13370300
C	-2.80654400	-1.47911000	-0.13838100
C	-4.06461600	-0.86783400	-0.02348600
H	-5.10382400	1.02439500	0.19530000
H	-3.06724400	2.36333100	0.20427500
H	-0.68429800	-1.18809700	-0.22005100
H	-2.76216800	-2.55981900	-0.22899200
C	-0.47495700	1.50798600	-0.02663900
N	-0.34546300	2.77936700	-0.05526000
H	-1.24128300	3.26412900	-0.09288600
Si	2.16795900	1.55974500	-0.01581200
H	2.33275300	2.33883200	-1.26570500
H	2.32462100	2.38789400	1.20318200
C	3.43603700	0.18270400	0.01076900
C	3.89798100	-0.35787600	1.22481300
C	3.96516500	-0.33769700	-1.18429900

C	4.84057300	-1.38632200	1.24587800
H	3.51920700	0.03088100	2.16805100
C	4.90837700	-1.36605400	-1.17007900
H	3.63903600	0.06708600	-2.14035900
C	5.34616700	-1.89248700	0.04665500
H	5.18367500	-1.79001600	2.19510500
H	5.30422400	-1.75372400	-2.10535500
H	6.08310100	-2.69155500	0.06063800
O	0.65711700	0.75826700	-0.00041700
O	-5.13514700	-1.70730400	-0.03704500
C	-6.43609400	-1.14852200	0.07625800
H	-7.12690100	-1.99249800	0.04019900
H	-6.56373100	-0.61536400	1.02724500
H	-6.65420700	-0.46496600	-0.75447500

Int2uncat

0 1

C	-3.59638000	-0.62730100	0.85136800
C	-2.24830400	-0.80621900	0.53912500
C	-1.61921700	-0.03369800	-0.44302300
C	-2.37757500	0.94690400	-1.10718000
C	-3.71791300	1.13161300	-0.81505600
C	-4.34042300	0.34307200	0.16743700
H	-4.04883800	-1.23698100	1.62466600
H	-1.69022300	-1.54665100	1.10647300
H	-1.88379700	1.55569500	-1.85694900
H	-4.31105400	1.88136800	-1.32902400
C	-0.17897200	-0.16701800	-0.81998300
N	0.51414900	-1.28281800	-0.41619100
H	0.00879300	-2.02184600	0.05483600
Si	2.21269800	-1.49229600	-0.90242500
H	2.51388200	-2.87381600	-0.43377400
H	2.30961900	-1.44213600	-2.38123700
C	3.41869900	-0.33081400	-0.06470600
C	3.40000600	1.06246400	-0.27261000
C	4.40620300	-0.86142900	0.78590300
C	4.33542500	1.88881600	0.34975100
H	2.63853300	1.49529900	-0.91402200
C	5.34486000	-0.03514500	1.40685500
H	4.44625600	-1.93357700	0.96663600
C	5.30976700	1.34240100	1.18876100
H	4.30464400	2.96216200	0.17998600
H	6.09995700	-0.46603800	2.05954600
H	6.03854000	1.98905400	1.67119400
O	0.39411400	0.69719300	-1.48867400
O	-5.65809700	0.60073300	0.38332100
C	-6.34648500	-0.15994700	1.36587500

H	-7.37303100	0.21008100	1.36351400
H	-6.34525900	-1.22970400	1.11989900
H	-5.91111700	-0.01663100	2.36326700

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C	4.07113600	0.73437100	0.20816200
C	2.77634400	1.24053300	0.13776600
C	1.67773200	0.39599600	-0.06382100
C	1.90230700	-0.98716800	-0.19527400
C	3.18459900	-1.50341900	-0.12673900
C	4.28074100	-0.64699700	0.07563400
H	4.90120600	1.41319800	0.36344600
H	2.63048400	2.31251300	0.23915500
H	1.05265900	-1.64290100	-0.34985500
H	3.37134400	-2.56775700	-0.22580900
C	0.30712800	0.91457900	-0.13949500
N	-0.13976700	2.13226600	-0.01374700
H	0.45958400	2.92698800	0.17489700
Si	-2.03075400	1.44380300	-0.42338700
H	-2.58496500	2.58139100	0.38288500
H	-2.03425600	1.81498400	-1.86168700
C	-3.41341700	0.18187200	-0.07523700
C	-3.37387100	-1.15911100	-0.50391200
C	-4.57146800	0.61255400	0.59399000
C	-4.44664700	-2.02318000	-0.28545800
H	-2.48815100	-1.53185600	-1.01100800
C	-5.65115900	-0.24584800	0.81768600
H	-4.62989000	1.63929800	0.95100100
C	-5.59019200	-1.56756300	0.37647700
H	-4.39258300	-3.05392800	-0.62862200
H	-6.53454300	0.11490500	1.33953800
H	-6.42579400	-2.24147700	0.55003800
O	-0.69674100	0.10521500	-0.37233500
O	5.49505900	-1.24929800	0.12788900
C	6.64980300	-0.44415600	0.33132400
H	6.60466500	0.08562200	1.29115600
H	7.49457300	-1.13437800	0.33825600
H	6.77984000	0.28216300	-0.48079000

Int1

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C	-0.60014000	0.36777500	-0.41569500
C	1.38103800	-0.75786100	0.02414800
C	0.46576100	1.26212300	-0.35655800
N	0.03669200	-0.86094200	-0.18793800

N	1.66914000	0.56623200	-0.07246000
C	0.36398000	2.71909000	-0.55293300
C	1.37748100	3.53224800	-1.09340500
C	-0.85913100	3.33424300	-0.21604200
C	1.17866500	4.90191500	-1.27662900
H	2.32901000	3.10306900	-1.37974300
C	-1.05577600	4.69855500	-0.40639500
H	-1.64842300	2.71734000	0.19724400
C	-0.03612100	5.49498800	-0.93462900
H	1.98057600	5.50347900	-1.69751700
H	-2.00925900	5.14389700	-0.13337000
H	-0.18800500	6.56139200	-1.07904100
C	2.32670100	-1.85553500	0.28695400
C	2.23845400	-3.05672400	-0.44283700
C	3.32978800	-1.74902500	1.26919400
C	3.11553200	-4.11001600	-0.19436400
H	1.48374300	-3.16496100	-1.21122600
C	4.20876500	-2.80330700	1.50961500
H	3.42422200	-0.83965800	1.84784600
C	4.10592000	-3.99002300	0.78197200
H	3.02644400	-5.02508500	-0.77327900
H	4.97228600	-2.69583100	2.27515200
H	4.78995100	-4.81203600	0.97362000
C	-0.72640600	-2.08816900	-0.12966000
C	-1.14422400	-2.67767000	-1.34192000
C	-1.08518300	-2.61423600	1.12571500
C	-1.93141700	-3.83196400	-1.26403200
C	-1.86613400	-3.77746700	1.14394500
C	-2.28667200	-4.38248900	-0.03518000
H	-2.27420700	-4.30626300	-2.17874600
H	-2.15751500	-4.20648900	2.09868000
H	-2.89784500	-5.28057700	0.00161100
C	2.98363700	1.13802000	0.12554000
C	3.95196100	1.00756300	-0.89426200
C	3.24352800	1.83387600	1.32773700
C	5.20857200	1.58419100	-0.67203100
C	4.51898000	2.38825200	1.49106300
C	5.49448800	2.26595500	0.50657200
H	5.97329400	1.49945600	-1.43879300
H	4.74840400	2.92731900	2.40575400
H	6.47693700	2.70581800	0.65615700
C	2.20891300	2.00912300	2.44059400
H	1.27403900	1.54335900	2.11696700
C	3.68608500	0.29394700	-2.21933200
H	2.67819800	-0.12920000	-2.18477800
C	-0.79002000	-2.08313000	-2.70391000
H	0.03319400	-1.37599000	-2.55765800
C	-0.69547900	-1.95343500	2.44493300

H	-0.06266800	-1.09006200	2.22080300
C	3.72387500	1.27483600	-3.40910800
H	4.70889500	1.74581300	-3.50918600
H	3.51349800	0.74118200	-4.34332700
H	2.97849700	2.06917400	-3.30178000
C	4.66966600	-0.87077000	-2.44857700
H	4.65241500	-1.58244000	-1.61821200
H	4.40618900	-1.40981800	-3.36607400
H	5.69840300	-0.50953900	-2.56399800
C	1.90906600	3.49920900	2.70294300
H	1.10931800	3.59411300	3.44644700
H	2.78998300	4.02087100	3.09623900
H	1.58921100	4.00968300	1.79104800
C	2.64385000	1.31673200	3.74848300
H	1.87721000	1.45780100	4.51914100
H	2.78683800	0.23881800	3.61672800
H	3.58144800	1.73469900	4.13344400
C	-1.93822300	-1.41636400	3.18200700
H	-2.48637500	-0.70375200	2.55810200
H	-2.62373000	-2.22768900	3.45455300
H	-1.64156400	-0.90604200	4.10637900
C	0.11882700	-2.90055300	3.34706000
H	-0.47038900	-3.77403600	3.65020400
H	1.01906800	-3.26183200	2.83937000
H	0.42802500	-2.37976000	4.26132900
C	-1.97297400	-1.27507600	-3.27318900
H	-2.85297000	-1.91441500	-3.41527800
H	-2.23540000	-0.46076500	-2.59324300
H	-1.70657000	-0.84482900	-4.24655200
C	-0.31112100	-3.14165500	-3.71514900
H	0.52262300	-3.73786900	-3.32539500
H	-1.11224600	-3.83496200	-3.99546000
H	0.02727100	-2.65051900	-4.63478800
Si	-4.16082800	0.69942600	-0.11064100
H	-3.52327200	1.32859500	1.07786000
H	-3.73554100	1.41288200	-1.33918200
H	-3.81714200	-0.74173100	-0.15343400
C	-6.04067000	0.85457600	0.02748300
C	-6.80519500	-0.10831600	0.71106700
C	-6.72394200	1.94670300	-0.53706900
C	-8.18972800	0.01721900	0.83590100
H	-6.31381600	-0.97513800	1.14950300
C	-8.10850200	2.07947400	-0.41664800
H	-6.16807900	2.70480900	-1.08577800
C	-8.84461600	1.11395700	0.27221100
H	-8.75815700	-0.74166800	1.36832900
H	-8.61308200	2.93271800	-0.86364000
H	-9.92331100	1.21295100	0.36524000

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C	-0.60397900	0.15013600	1.20617800
C	-2.19126000	-0.54281400	-0.26686100
C	-0.83771700	1.16604400	0.31059800
N	-1.47340100	-0.88567000	0.83923600
N	-1.81512200	0.72309700	-0.59811800
C	-0.22099500	2.51300900	0.26477200
C	-0.95810600	3.64515100	0.64374600
C	1.12912700	2.65606200	-0.09099800
C	-0.36358500	4.90542100	0.65050400
H	-1.99055000	3.53242800	0.95784300
C	1.71946300	3.92104500	-0.07736300
H	1.70409800	1.78057500	-0.38713200
C	0.97785900	5.04486000	0.28797700
H	-0.94392300	5.77472900	0.94780000
H	2.76642800	4.02229100	-0.34817400
H	1.44451200	6.02630900	0.29844400
C	-3.16484700	-1.38877300	-0.99141300
C	-3.98897900	-2.31177400	-0.31756700
C	-3.28773600	-1.29984700	-2.39158700
C	-4.89696900	-3.10376200	-1.01665800
H	-3.92813400	-2.42119400	0.75400700
C	-4.19494600	-2.09689800	-3.08520100
H	-2.67110500	-0.61306800	-2.94990300
C	-5.00680200	-3.00285700	-2.40328000
H	-5.51986600	-3.80330000	-0.46683300
H	-4.25720500	-2.00888000	-4.16583700
H	-5.71315900	-3.62476000	-2.94570000
C	-1.59593700	-2.14686700	1.56077500
C	-2.40224600	-2.18099100	2.72343500
C	-0.92517900	-3.28085400	1.05927900
C	-2.57318200	-3.42532100	3.34116200
C	-1.14130700	-4.49528100	1.72470900
C	-1.96363400	-4.57357000	2.84185100
H	-3.19250300	-3.49483600	4.23011600
H	-0.64586400	-5.38900200	1.35827600
H	-2.11788900	-5.52803600	3.33810300
C	-2.36611100	1.52887400	-1.68309100
C	-3.65681000	2.08060000	-1.52604500
C	-1.59468100	1.71776700	-2.85471400
C	-4.18425900	2.80256500	-2.60390300
C	-2.18310200	2.44901400	-3.89415400
C	-3.46338100	2.97970600	-3.77921600
H	-5.17725700	3.23316800	-2.51648100
H	-1.62012700	2.60324700	-4.80920700
H	-3.89627900	3.54019500	-4.60343600

C	-0.18364700	1.16519400	-3.04596100
H	0.18045800	0.81551800	-2.08060700
C	-4.50406600	1.93644000	-0.26211100
H	-3.91289100	1.41093200	0.49546300
C	-3.09442400	-0.95415600	3.32639700
H	-2.69229900	-0.05910000	2.84281400
C	0.02650200	-3.24222500	-0.13087800
H	0.13119700	-2.20391700	-0.45230400
C	-4.88723300	3.30946000	0.32810300
H	-5.56630900	3.85482000	-0.33677400
H	-5.40171300	3.17634700	1.28662900
H	-4.01125900	3.94318900	0.49463700
C	-5.77998900	1.10842400	-0.52108000
H	-5.55130600	0.11920200	-0.92541900
H	-6.34008900	0.97654400	0.41212100
H	-6.43900300	1.61842100	-1.23331000
C	0.80445800	2.24982900	-3.51748500
H	1.82135800	1.84835000	-3.46434300
H	0.61558800	2.54887200	-4.55548400
H	0.75658800	3.14298200	-2.88823300
C	-0.13007000	-0.03698600	-4.01396300
H	0.88600700	-0.44445400	-4.04089200
H	-0.78586300	-0.85575500	-3.70251400
H	-0.41876200	0.25940700	-5.03008800
C	1.43817500	-3.72126500	0.26196000
H	1.84386100	-3.12559600	1.08512000
H	1.43350900	-4.77541200	0.56547700
H	2.10175500	-3.61318800	-0.60096400
C	-0.49098000	-4.04800100	-1.33871400
H	-0.52965900	-5.12138500	-1.11534600
H	-1.49354100	-3.73330100	-1.64683800
H	0.19531000	-3.89847900	-2.17903500
C	-2.80073000	-0.81948900	4.83426700
H	-3.27685300	-1.61980700	5.41231300
H	-1.72720800	-0.83876900	5.03647700
H	-3.19768500	0.13246400	5.20477100
C	-4.62071800	-0.96573800	3.09608600
H	-4.88421300	-0.93349300	2.03426200
H	-5.07942600	-1.86276700	3.52894400
H	-5.07798900	-0.09382900	3.57837400
Si	0.60606600	0.07705900	2.71071700
H	-0.37933400	0.54305800	3.76018100
H	0.85993000	-1.32565800	3.11586400
H	1.83545900	-0.54667900	1.20159400
C	1.95412000	1.37109300	3.00792100
C	1.61030300	2.53713300	3.71600800
C	3.30280600	1.19380100	2.65289800
C	2.56739400	3.50320300	4.03188400

H	0.57982800	2.69301200	4.02598500
C	4.26717500	2.14498600	2.98738400
H	3.59834800	0.30404100	2.10617200
C	3.90043800	3.30741600	3.66946300
H	2.27348100	4.40291300	4.56724200
H	5.30586500	1.97829300	2.71244400
H	4.65080700	4.05292200	3.92172000
H	2.08487200	-0.51839900	0.32318400
N	2.21634400	-0.45763400	-1.10677300
H	1.28377700	-0.72600900	-1.42701300
C	3.06898100	-1.26624100	-1.78138700
C	4.53190200	-1.10196700	-1.46109300
C	5.02719200	-0.05768600	-0.66335700
C	5.44441800	-2.01768700	-1.99100100
C	6.38574800	0.05698300	-0.39705400
H	4.33404900	0.67274200	-0.25992900
C	6.81236600	-1.92023600	-1.73132100
H	5.05518200	-2.81331000	-2.61825500
C	7.28796400	-0.87687100	-0.92778700
H	6.77785400	0.86534300	0.21365400
H	7.49074200	-2.65202100	-2.15633600
O	2.72248400	-2.11821300	-2.63118800
O	8.60469800	-0.67866200	-0.60699500
C	9.55998500	-1.58921000	-1.12075200
H	10.52935500	-1.25095100	-0.74825200
H	9.37526200	-2.61350300	-0.76930600
H	9.57404600	-1.58691300	-2.21922400

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C	0.58319300	0.10020600	-0.63920900
C	2.64583400	-0.61472500	0.14378200
C	1.47854600	1.16217000	-0.59255000
N	1.37356900	-0.97139100	-0.19197800
N	2.73230700	0.71843100	-0.10529500
C	1.18656800	2.56187200	-0.95588100
C	2.05835000	3.37304600	-1.70252700
C	-0.05538300	3.09798900	-0.56674100
C	1.70154800	4.67660000	-2.04875600
H	3.01988900	2.98766500	-2.02037100
C	-0.41104900	4.39783400	-0.92225100
H	-0.72140800	2.49560100	0.04241200
C	0.46403600	5.19483700	-1.66398000
H	2.39193900	5.28406800	-2.62874400
H	-1.37311300	4.79177300	-0.60461600
H	0.18660300	6.20988000	-1.93668000
C	3.69815200	-1.48642000	0.69336800

C	3.88132500	-2.79188300	0.19817200
C	4.53687300	-1.05154700	1.73756300
C	4.86028500	-3.62792900	0.73090300
H	3.26058000	-3.15493800	-0.60994900
C	5.51859600	-1.88920000	2.26246700
H	4.42216600	-0.05504900	2.14217000
C	5.68521800	-3.18248100	1.76473800
H	4.98084200	-4.62979800	0.32819600
H	6.14960000	-1.52835800	3.06998800
H	6.44879900	-3.83558500	2.17790400
C	0.80040800	-2.29368800	-0.07770100
C	0.70832800	-3.08401700	-1.24467300
C	0.28296900	-2.70998700	1.16263400
C	0.03767400	-4.30772200	-1.14445900
C	-0.37123800	-3.94952700	1.20546100
C	-0.50503700	-4.73525100	0.06561000
H	-0.06107300	-4.93756100	-2.02314200
H	-0.78295300	-4.29933900	2.14812100
H	-1.02594000	-5.68760800	0.11957900
C	3.91318600	1.53158400	0.10010000
C	4.99738900	1.40919300	-0.79788400
C	3.93085900	2.43987100	1.18307900
C	6.12147300	2.21256600	-0.57027500
C	5.08475100	3.21394600	1.35789500
C	6.17105800	3.10403300	0.49616800
H	6.97068600	2.13789800	-1.24346300
H	5.12823800	3.91745600	2.18415100
H	7.05484900	3.71676000	0.65296800
C	2.76801600	2.61628300	2.16125500
H	1.93755100	1.98744800	1.83015300
C	5.00185500	0.45909500	-1.99579000
H	4.06063400	-0.09817900	-1.99713200
C	1.32503800	-2.64304600	-2.57357400
H	2.08938500	-1.89057000	-2.34752900
C	0.41713000	-1.88387300	2.43916800
H	0.99606700	-0.98613100	2.20478800
C	5.07654500	1.22250800	-3.33389600
H	5.99698000	1.81307300	-3.40888700
H	5.06688700	0.51443300	-4.17080500
H	4.22851100	1.90238400	-3.46248200
C	6.14997800	-0.56633400	-1.90267200
H	6.11821900	-1.12479300	-0.96315500
H	6.08251000	-1.28338600	-2.72926800
H	7.12810800	-0.07586100	-1.97176200
C	2.26039000	4.07269800	2.17643700
H	1.36626000	4.14768400	2.80527900
H	3.01410000	4.75484900	2.58832700
H	1.99846600	4.41717800	1.17309000

C	3.14253900	2.17294600	3.59064100
H	2.28756800	2.31687800	4.26102400
H	3.42301200	1.11516000	3.63554000
H	3.97959800	2.75950300	3.98761300
C	-0.94987900	-1.40531400	2.96404500
H	-1.43038700	-0.72337100	2.25667400
H	-1.62296400	-2.24930500	3.15969800
H	-0.81832200	-0.86220600	3.90778000
C	1.19275200	-2.65878700	3.52352700
H	0.64421400	-3.54911500	3.85337400
H	2.17426600	-2.98338900	3.16190700
H	1.34581600	-2.02275800	4.40337900
C	0.29273600	-1.96063700	-3.49116300
H	-0.52494600	-2.64709300	-3.74060300
H	-0.12898100	-1.08019000	-2.99992900
H	0.76905300	-1.64543600	-4.42789400
C	2.03087700	-3.79438700	-3.31444000
H	2.75488100	-4.31489900	-2.67651100
H	1.31896100	-4.53978400	-3.68650100
H	2.56863700	-3.40055200	-4.18445600
Si	-3.48438400	-0.89717000	-1.68087400
H	-2.41025800	-1.72600300	-2.27360300
H	-4.22676800	-0.24286600	-2.79433600
C	-4.71804100	-1.97059100	-0.75657300
C	-6.05404800	-2.06106600	-1.18282100
C	-4.32597700	-2.74194300	0.35335900
C	-6.96762100	-2.89034100	-0.52911300
H	-6.38882600	-1.47086000	-2.03314800
C	-5.23538900	-3.56966600	1.01151700

Int3

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C	0.44707600	-0.16372600	-0.18794900
C	2.65536200	-0.66144300	0.30469200
C	1.29947500	0.53633700	-1.03560600
N	1.34438300	-0.89938000	0.60078400
N	2.64740800	0.23682200	-0.71585300
C	0.87694400	1.44013500	-2.12225700
C	1.57970200	1.62082300	-3.32822100
C	-0.34173700	2.13012500	-1.96688600
C	1.09044100	2.46492100	-4.32615900
H	2.51229400	1.09997100	-3.50119000
C	-0.83072700	2.96554100	-2.96678800
H	-0.90115700	2.00385100	-1.04816500
C	-0.11549000	3.14352900	-4.15337300
H	1.65603400	2.58192500	-5.24721100
H	-1.77390400	3.48342400	-2.81367500

H	-0.49530100	3.79835500	-4.93308000
C	3.84322700	-1.23724300	0.96074700
C	3.87048000	-2.59404300	1.33764400
C	4.97672400	-0.45087500	1.24505100
C	4.98617000	-3.13924200	1.96926700
H	3.01608200	-3.22636600	1.13898200
C	6.09175500	-1.00203400	1.87306200
H	4.98931500	0.59672700	0.97701200
C	6.10412100	-2.34865300	2.23952000
H	4.97928400	-4.18993800	2.24545800
H	6.95049900	-0.37014100	2.08226500
H	6.97338500	-2.77604400	2.73145600
C	0.87226700	-1.83413400	1.60152900
C	0.34990400	-3.07308500	1.16670700
C	0.91670900	-1.47375000	2.96310200
C	-0.09574300	-3.96616600	2.14871800
C	0.45772600	-2.40923400	3.89939100
C	-0.03774500	-3.64596900	3.50175000
H	-0.49997200	-4.92738600	1.84458000
H	0.48335100	-2.15821600	4.95604100
H	-0.38975100	-4.35650300	4.24509800
C	3.82965900	0.79398100	-1.33861400
C	4.58481300	-0.00930600	-2.22160600
C	4.17052700	2.13695900	-1.06095300
C	5.71381700	0.56804100	-2.81582900
C	5.31043400	2.65670400	-1.68638500
C	6.07766400	1.88487900	-2.55317200
H	6.31424500	-0.02545700	-3.49923100
H	5.59846200	3.68556500	-1.49080900
H	6.95768900	2.31113300	-3.02737800
C	3.36518400	3.03525300	-0.12053500
H	2.49919700	2.47090000	0.23608600
C	4.21991600	-1.45228800	-2.56969000
H	3.34591500	-1.73873500	-1.97821100
C	0.25522800	-3.48021300	-0.30460300
H	0.59650000	-2.63952200	-0.91400400
C	1.41354500	-0.11643800	3.45424500
H	1.71163600	0.47436400	2.58268000
C	3.82710700	-1.59670800	-4.05431700
H	4.65671900	-1.32409400	-4.71724300
H	3.55526800	-2.63625700	-4.27113900
H	2.96920700	-0.96655300	-4.30910200
C	5.35826700	-2.43006900	-2.21586500
H	5.64874800	-2.34803200	-1.16459400
H	5.03809600	-3.46171800	-2.40251900
H	6.24873900	-2.24651700	-2.82863000
C	2.82815300	4.28258700	-0.85170000
H	2.19050400	4.86539500	-0.17711600

H	3.64550500	4.93574600	-1.18034800
H	2.23625100	4.00904700	-1.72872800
C	4.18494400	3.45630200	1.11656700
H	3.57645200	4.09227800	1.76985900
H	4.51399300	2.59390300	1.70620000
H	5.07604200	4.02868800	0.83329600
C	0.29010600	0.66197000	4.16715900
H	-0.58724600	0.78078400	3.52469900
H	-0.03209300	0.15110400	5.08213200
H	0.64328500	1.66007600	4.45374500
C	2.64449300	-0.25041600	4.37254800
H	2.39690700	-0.79549200	5.29118400
H	3.46358500	-0.78065100	3.87788900
H	3.00746900	0.74185600	4.66652700
C	-1.20205800	-3.76513500	-0.71799500
H	-1.61757200	-4.61633900	-0.16454300
H	-1.84345500	-2.89539600	-0.55193400
H	-1.24162200	-4.01559200	-1.78507300
C	1.15036200	-4.69485200	-0.62615700
H	2.20856400	-4.49887500	-0.41872800
H	0.85511600	-5.57746000	-0.04630400
H	1.06282500	-4.95343500	-1.68799300
Si	-5.29553800	-1.52639900	-1.25365200
H	-4.74261000	-1.40080100	-2.62410000
H	-4.81296600	-2.76110000	-0.58688400
C	-7.16873400	-1.55896700	-1.40272800
C	-8.00685300	-1.39216900	-0.28450700
C	-7.77761600	-1.78575000	-2.64892800
C	-9.39500300	-1.45289000	-0.40612300
H	-7.56862700	-1.20363200	0.69315000
C	-9.16691600	-1.85249800	-2.77718400
H	-7.15919100	-1.90594800	-3.53651900
C	-9.97802900	-1.68601500	-1.65432300
H	-10.02352800	-1.31833200	0.47096100
H	-9.61479800	-2.02822200	-3.75224100
H	-11.05994700	-1.73445700	-1.75036600
N	-2.80876200	-0.61349900	-0.49911000
C	-3.70337900	0.14618300	-0.00944400
O	-5.01187900	-0.16052400	-0.27907100
C	-3.56562300	1.36555900	0.82965500
C	-4.68358500	2.14334300	1.15316500
C	-2.30701200	1.77157600	1.31179500
C	-4.56645200	3.29967500	1.92590800
H	-5.65866000	1.83947000	0.79042800
C	-2.17926200	2.92053400	2.07795400
H	-1.42259300	1.18167300	1.07927100
C	-3.30755100	3.69511900	2.39175400
H	-5.45479200	3.87790900	2.15342700

H	-1.21200400	3.24146400	2.45176400
H	-1.82759200	-0.36469300	-0.30343000
O	-3.07167200	4.80406500	3.15050500
C	-4.17437800	5.62538500	3.50058800
H	-3.76245700	6.44105900	4.09779400
H	-4.66745100	6.04006500	2.61148000
H	-4.91359900	5.07591500	4.09823100

TS2

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C	0.62601700	0.09250800	-0.41429400
C	2.59545300	-0.91638200	0.09542600
C	1.65550200	0.91598600	-0.83207800
N	1.24269000	-1.02325700	0.13212700
N	2.87144800	0.28577300	-0.48110200
C	1.48498700	2.18246200	-1.57106700
C	2.51534900	2.89409900	-2.21506600
C	0.17016500	2.68733200	-1.67789000
C	2.24306400	4.06836500	-2.91995400
H	3.53729300	2.54385300	-2.18112500
C	-0.09078700	3.85890800	-2.38059100
H	-0.65600300	2.15270700	-1.21939200
C	0.94272500	4.56149400	-3.00449500
H	3.06064800	4.59367300	-3.40686000
H	-1.11321500	4.22142100	-2.43961500
H	0.73509100	5.47605800	-3.55320100
C	3.56887500	-1.92977600	0.54158400
C	3.37375000	-3.28283800	0.20734200
C	4.70107300	-1.58494100	1.30136700
C	4.27991100	-4.25567300	0.62324300
H	2.51324600	-3.57486400	-0.38036900
C	5.60604300	-2.56185100	1.71181800
H	4.87654500	-0.55339400	1.57480000
C	5.40005800	-3.90086100	1.37655900
H	4.10923200	-5.29336800	0.35145900
H	6.47124400	-2.27234000	2.30137700
H	6.10564600	-4.66091900	1.69988600
C	0.48242700	-2.14990600	0.64629800
C	-0.11619600	-3.02590900	-0.28430100
C	0.32896800	-2.29435500	2.03766000
C	-0.86028100	-4.09379700	0.22936900
C	-0.41849000	-3.38872800	2.49099400
C	-1.00463800	-4.28130900	1.60080500
H	-1.34253900	-4.78284600	-0.45714200
H	-0.55664500	-3.52986300	3.55887800
H	-1.58898400	-5.11730500	1.97559300
C	4.21255100	0.81369700	-0.63801200

C	5.00505000	0.35015500	-1.70847700
C	4.66474400	1.78656500	0.28156000
C	6.29342600	0.88490000	-1.83358400
C	5.96136900	2.28329200	0.10246300
C	6.76999900	1.83883600	-0.93979400
H	6.92911200	0.55119500	-2.64837000
H	6.34061300	3.03398600	0.78958300
H	7.77251300	2.24094200	-1.05831100
C	3.80872000	2.32814500	1.42795300
H	2.84647900	1.80730700	1.41568700
C	4.50968200	-0.66226900	-2.73862900
H	3.51925100	-1.00965900	-2.43000500
C	-0.01305200	-2.83819900	-1.79712900
H	0.73149700	-2.06052900	-1.99684100
C	0.88811200	-1.30219300	3.05276500
H	1.44173400	-0.52866300	2.51045800
C	4.34673800	-0.00859500	-4.12632500
H	5.30692200	0.35510600	-4.51086700
H	3.95514700	-0.73926800	-4.84328000
H	3.65326600	0.83769300	-4.09224700
C	5.42607800	-1.89866100	-2.81797400
H	5.53826900	-2.38019200	-1.84174000
H	5.00459000	-2.63260200	-3.51432600
H	6.42575400	-1.63657900	-3.18341900
C	3.51682500	3.83230400	1.24590900
H	2.84713100	4.18258400	2.03970700
H	4.43774300	4.42489000	1.30279400
H	3.03959900	4.03628100	0.28398300
C	4.45074100	2.07801100	2.80782300
H	3.79893300	2.46889500	3.59714900
H	4.60717800	1.01237100	3.00584900
H	5.41958200	2.58206800	2.89996900
C	-0.25457200	-0.59360000	3.80740400
H	-0.94650400	-0.10661600	3.11458300
H	-0.82754800	-1.30259200	4.41628800
H	0.15083300	0.17193700	4.47927600
C	1.87057500	-1.96993900	4.03434300
H	1.37043400	-2.73130200	4.64399500
H	2.70171500	-2.45235600	3.50973300
H	2.28624100	-1.22183400	4.71984800
C	-1.35425700	-2.33968500	-2.37393900
H	-2.13650500	-3.09777900	-2.24611600
H	-1.68606400	-1.42424800	-1.87476900
H	-1.25033400	-2.14244300	-3.44800700
C	0.45496600	-4.11413900	-2.52409000
H	1.41835000	-4.47915900	-2.14787400
H	-0.27034000	-4.92931400	-2.42485400
H	0.56958500	-3.90973500	-3.59478600

Si	-4.55625400	-0.29001200	-0.65076400
H	-4.19520300	-0.05483100	-2.07451900
H	-4.06570800	-1.61692600	-0.19077000
C	-6.44302700	-0.31083800	-0.61949900
C	-7.18137700	-0.22660700	0.57979000
C	-7.18045600	-0.44690900	-1.80322300
C	-8.56893600	-0.28144000	0.59405200
H	-6.65604300	-0.10399900	1.52434600
C	-8.57886700	-0.50757400	-1.81585900
H	-6.65826200	-0.50187800	-2.75710000
C	-9.27767600	-0.42520900	-0.60815600
H	-9.13118100	-0.21210100	1.52094800
H	-9.10219300	-0.61056400	-2.76034200
N	-2.03986000	0.41728600	-0.17220700
C	-2.79719700	1.13165200	0.52917600
O	-4.19379000	0.96058600	0.43365200
C	-2.47301800	2.21716000	1.51462000
C	-3.48155100	2.93998200	2.17143800
C	-1.13527300	2.53524400	1.79421800
C	-3.15933200	3.95045700	3.07828700
H	-4.51670400	2.70056800	1.95923500
C	-0.81304900	3.54369900	2.70026700
H	-0.34915200	1.98105900	1.29199200
C	-1.82471300	4.25759600	3.34742200
H	-3.95499800	4.50018400	3.57552700
H	0.23060800	3.77616300	2.90119300
H	-1.57427700	5.04568200	4.05338200
H	-0.66766100	0.29078100	-0.28036400
O	-10.64144100	-0.47016000	-0.49125300
C	-11.40700700	-0.60837400	-1.67445500
H	-11.17642200	-1.54477000	-2.20081900
H	-12.45198200	-0.62250800	-1.35737000
H	-11.24923400	0.23433300	-2.36139500

aNHCcation

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N	0.84113900	0.00510600	-0.07459700
N	-1.20601300	-0.76241300	-0.02736000
C	1.97552800	0.92089100	-0.07956600
C	2.77836100	1.00061900	1.07982200
C	-3.21948100	-0.82937100	1.38683300
C	0.92923400	-1.39287900	-0.18454200
C	2.23279100	1.66858400	-1.24944200
C	-2.64924700	-0.91101000	0.10116500
C	-0.35915200	-1.84585100	-0.14933500
H	-0.74708100	-2.84869300	-0.21913400
C	2.16660400	-3.44959100	0.37871300

H	1.32017800	-3.74333100	0.99293800
C	-0.46811500	0.37336700	0.01907600
C	-1.00140300	1.73842300	0.14053100
C	2.53262900	0.18914000	2.35336700
H	1.66296100	-0.45727300	2.19435300
C	3.33815600	2.52813300	-1.22307900
H	3.56918300	3.12012200	-2.10314100
C	3.27015200	-1.82975400	-1.04273200
H	3.28265600	-0.88158700	-1.56520400
C	-4.60371500	-1.02197600	1.47804400
H	-5.08358700	-0.96445300	2.45003700
C	4.14571800	2.63700000	-0.09561000
H	4.99708800	3.31136800	-0.10163800
C	-2.41068700	-0.58441500	2.65786400
H	-1.36581700	-0.41032400	2.37924600
C	-5.37172500	-1.29903700	0.35174000
H	-6.44277900	-1.44957000	0.45054100
C	2.15126900	-2.20697200	-0.28179100
C	-0.92594900	3.96289700	1.10968300
H	-0.45491300	4.67550500	1.77974900
C	3.86651900	1.88099400	1.03839600
H	4.50676600	1.97214800	1.91023900
C	-3.39370200	-1.20258700	-1.06155000
C	3.73247500	-0.72517100	2.67858200
H	3.98595900	-1.37769200	1.83907100
H	3.49854000	-1.35463100	3.54414600
H	4.62191600	-0.13725100	2.93068600
C	4.37338000	-2.67675700	-1.13675200
H	5.23001100	-2.37293000	-1.73095600
C	-2.13470400	2.11832500	-0.60154500
H	-2.60485500	1.41460900	-1.27656600
C	1.39161400	1.58645000	-2.52361100
H	0.55289400	0.90447900	-2.34716200
C	2.21568600	1.09200800	3.56398100
H	3.04652900	1.76968800	3.78763700
H	2.04373200	0.47592900	4.45334400
H	1.32030900	1.70255000	3.40552500
C	4.37716200	-3.90945000	-0.48160800
H	5.23907500	-4.56539600	-0.55902900
C	-0.40043300	2.67795000	0.99700500
H	0.47183300	2.40715200	1.57678000
C	3.26892000	-4.29423300	0.27573500
H	3.26589300	-5.24746000	0.79577500
C	-2.05216200	4.33092100	0.37083200
H	-2.45884400	5.33376900	0.46069600
C	-2.65271300	3.40560300	-0.48518000
H	-3.52409000	3.68608200	-1.06888900
C	-4.77082600	-1.39383400	-0.90044400

H	-5.38103100	-1.62211500	-1.76855000
C	2.19934000	1.01049100	-3.70526800
H	3.06171400	1.64145600	-3.94604600
H	1.56851800	0.95648400	-4.59933200
H	2.56904200	0.00115700	-3.49644900
C	-2.89361100	0.66776100	3.41528400
H	-2.85999700	1.55920800	2.78094100
H	-2.25821200	0.84563900	4.28991600
H	-3.92117100	0.54889700	3.77549800
C	-2.76671800	-1.34327600	-2.44847100
H	-1.72581900	-1.00391200	-2.39449900
C	0.79700400	2.95932300	-2.89870300
H	0.22019100	3.39080500	-2.07562200
H	0.13444400	2.85650800	-3.76516100
H	1.58236300	3.67307700	-3.17015000
C	-3.47114000	-0.47310400	-3.50800400
H	-4.50448100	-0.79348200	-3.67659400
H	-2.94433500	-0.55248200	-4.46496500
H	-3.49344500	0.58464200	-3.22337700
C	-2.43171800	-1.82785200	3.57055900
H	-3.44653700	-2.05306900	3.91595900
H	-1.80870100	-1.65862200	4.45572200
H	-2.05239700	-2.71472000	3.05090700
C	-2.74676100	-2.82034100	-2.89526000
H	-2.20973500	-3.45604800	-2.18267900
H	-2.25740600	-2.91720900	-3.87049200
H	-3.76390500	-3.21640600	-2.98870800

H2

0 1			
H	0.00000000	0.00000000	0.37139400
H	0.00000000	0.00000000	-0.37139400

Pdt

0 1			
C	-0.67448200	-1.01077200	-0.00028500
C	0.71096900	-1.15156300	-0.00024100
C	1.54585600	-0.02480700	-0.00006900
C	0.96636200	1.25951200	0.00003600
C	-0.41045700	1.40463000	0.00004000
C	-1.24238100	0.27166400	-0.00039300
H	-1.29728400	-1.89731000	-0.00024100
H	1.15161300	-2.14346700	-0.00023100
H	1.60635400	2.13596800	0.00022300
H	-0.87247800	2.38634900	0.00018500
C	2.96905400	-0.17850200	0.00014500

N	4.12640000	-0.30295400	0.00024700
O	-2.57593000	0.52441800	-0.00032700
C	-3.47846400	-0.57459700	0.00056600
H	-4.47790500	-0.13731200	0.00122600
H	-3.35386700	-1.19616200	-0.89516000
H	-3.35253100	-1.19612000	0.89609200

PhSiH₂O

-1 1

Si	-2.03454700	-0.44656500	0.00027400
H	-2.20871500	-1.40931500	1.18238400
H	-2.20906500	-1.41107300	-1.18034900
C	-0.11392400	-0.20957600	-0.00010700
C	0.40525700	1.09625400	0.00004200
C	0.81479300	-1.26384000	-0.00022600
C	1.78151000	1.34269200	0.00013100
H	-0.30801000	1.91904100	0.00005600
C	2.19366900	-1.03450800	-0.00013700
H	0.45332900	-2.29357700	-0.00045300
C	2.68331500	0.27516100	0.00006000
H	2.15532400	2.36686600	0.00024300
H	2.88971200	-1.87378400	-0.00022500
H	3.75699500	0.46008800	0.00016800
O	-2.82920500	0.90707200	-0.00052900

PhSiH₂OH

0 1

C	2.18070900	-1.05028600	-0.17436100
C	0.80182900	-1.25283100	-0.09541000
C	-0.08045200	-0.17503800	0.09280400
C	0.46319600	1.11892400	0.18697700
C	1.83987100	1.32660000	0.10226500
C	2.70091500	0.24099600	-0.07487300
H	2.84671300	-1.89679200	-0.32084400
H	0.40876500	-2.26320900	-0.19032100
H	-0.19801500	1.97282300	0.31293800
H	2.24199200	2.33411200	0.17238300
H	3.77395300	0.40229700	-0.14030600
Si	-1.91693300	-0.47002100	0.24823200
H	-2.37062200	-0.48330400	1.67262900
H	-2.22810200	-1.81384100	-0.32163700
O	-2.68118400	0.77420200	-0.56283200
H	-3.62454800	0.88440200	-0.38184400

Int4

0 1

C	-3.10096800	-3.13839300	0.20830200
C	-1.87166200	-2.50091900	0.21623300
C	-1.77211200	-1.10952100	0.03145800
C	-2.95804500	-0.38330700	-0.15345600
C	-4.20090700	-1.01216600	-0.17111900
C	-4.27869100	-2.39962000	0.00940100
H	-3.17983400	-4.21046400	0.35700200
H	-0.98104000	-3.09310200	0.39208100
H	-2.90203500	0.69018700	-0.28881700
H	-5.09409700	-0.41729600	-0.32298500
C	-0.45668600	-0.42042600	0.02706500
N	0.71866400	-0.90931400	0.01421700
Si	0.83044900	1.88335300	0.04279400
H	1.62266900	1.62686000	1.26784200
H	1.60661900	1.66580200	-1.20194500
C	0.22318400	3.65369400	0.06932600
C	-0.03248300	4.35334700	-1.12423500
C	0.01859400	4.33072200	1.28547500
C	-0.48748700	5.67221200	-1.10559200
H	0.12888200	3.86385000	-2.08275000
C	-0.43614600	5.64967500	1.31077000
H	0.21982500	3.82307700	2.22676200
C	-0.69098400	6.32161700	0.11369300
H	-0.67886800	6.19453700	-2.03953400
H	-0.58760500	6.15422300	2.26162800
H	-1.04199400	7.35031500	0.13073600
O	-0.59504800	0.93634800	0.03484800
Si	1.54872300	-2.41534700	-0.08947100
H	1.24727900	-3.33036000	1.05346700
H	1.15189800	-3.12671600	-1.34205000
C	3.40065200	-2.11494000	-0.06676400
C	3.98597200	-1.03404800	-0.75001100
C	4.25141300	-3.00046100	0.61673900
C	5.36876300	-0.84812600	-0.75422100
H	3.35254300	-0.32429600	-1.27649000
C	5.63621400	-2.82102700	0.61362800
H	3.82873200	-3.83861700	1.16772700
C	6.19691600	-1.74335200	-0.07315300
H	5.80117100	-0.00445300	-1.28652400
H	6.27531300	-3.51671600	1.15175000
H	7.27437800	-1.59854500	-0.07459500
O	-5.43293100	-3.11739200	0.01315400
C	-6.66090800	-2.42811800	-0.17795800
H	-6.69259300	-1.92696400	-1.15382100
H	-7.43964100	-3.19145900	-0.13801000
H	-6.83456600	-1.68946500	0.61495300

TS3

0 1

C	0.32912900	4.12523500	-0.66048000
C	-0.11842000	2.82653900	-0.82543800
C	0.61104600	1.74130400	-0.30003700
C	1.80972800	2.00866800	0.37958500
C	2.26160600	3.31194500	0.56317300
C	1.51892500	4.38162600	0.04237000
H	-0.22119200	4.96486200	-1.07198500
H	-1.02690900	2.65038100	-1.38880600
H	2.39006900	1.18285800	0.77540900
H	3.18471200	3.48315000	1.10431700
C	0.15970900	0.35185100	-0.47084400
N	-1.05385500	-0.05505500	-0.67530500
Si	0.94140300	-2.24556300	-0.29420700
H	0.04631400	-2.52694500	0.85283300
H	0.37851300	-2.73523300	-1.57390800
C	2.63476300	-2.96385200	-0.00662400
C	3.11076000	-3.18642200	1.29879300
C	3.46954200	-3.30809900	-1.08597100
C	4.37989900	-3.72196800	1.51921200
H	2.48293400	-2.94394600	2.15370800
C	4.73935800	-3.84293300	-0.86948900
H	3.12440800	-3.16053700	-2.10709100
C	5.19551400	-4.04911500	0.43419200
H	4.73045900	-3.88833400	2.53434800
H	5.37047000	-4.10280300	-1.71514800
H	6.18331700	-4.46947400	0.60412200
O	1.16074800	-0.54653600	-0.40377000
Si	-2.78328100	0.58079100	-0.91417200
H	-2.70097200	1.69836100	0.09906800
H	-3.06343500	1.35572600	-2.15989400
C	-4.17207200	-0.44246100	-0.13581300
C	-4.72490400	-1.59527000	-0.72143300
C	-4.72099300	0.00108400	1.08194300
C	-5.78773200	-2.27099200	-0.12207600
H	-4.30651900	-1.96235300	-1.65450200
C	-5.77918500	-0.67675200	1.69116700
H	-4.31440400	0.88991900	1.55811500
C	-6.31623900	-1.81447300	1.08798900
H	-6.20273800	-3.15726300	-0.59640600
H	-6.18321600	-0.31686900	2.63449600
H	-7.14093400	-2.34469500	1.55846000
H	-1.44161800	-0.89370700	-1.41129400
H	-2.42912400	-0.92514500	-2.06865900
O	1.86552600	5.68858900	0.15395000

C	3.06406400	6.02015000	0.84371600
H	3.94254500	5.58060900	0.35468400
H	3.13573700	7.10817700	0.80720000
H	3.02766000	5.69262100	1.89032900

PhSiOSiPh

0 1

C	3.84376500	-1.44909300	-1.20842900
C	3.06281300	-0.29299200	-1.20858100
C	2.66031600	0.31355200	-0.00461300
C	3.07934900	-0.27502100	1.20261900
C	3.86039000	-1.43107200	1.20899500
C	4.24234200	-2.01994700	0.00193400
H	4.14430700	-1.90237500	-2.14958100
H	2.76581300	0.14427700	-2.15976300
H	2.79536500	0.17642400	2.15114700
H	4.17387600	-1.87028900	2.15259200
H	4.85288100	-2.91933500	0.00443500
Si	1.61005900	1.85951100	-0.00862900
H	1.93194700	2.66363700	1.20331900
H	1.92135500	2.65081200	-1.23171700
O	0.00001000	1.48773200	-0.00004900
Si	-1.61004300	1.85950800	0.00824800
H	-1.92147900	2.65107000	1.23112900
H	-1.93179700	2.66337000	-1.20391300
C	-2.66030500	0.31355100	0.00448200
C	-3.06328600	-0.29237300	1.20860400
C	-3.07887000	-0.27563100	-1.20261200
C	-3.84426100	-1.44846100	1.20873500
H	-2.76666000	0.14537600	2.15968100
C	-3.85992700	-1.43167100	-1.20870400
H	-2.79449700	0.17532500	-2.15125600
C	-4.24237000	-2.01992300	-0.00149300
H	-4.14517600	-1.90125900	2.15000100
H	-4.17305000	-1.87136500	-2.15219900
H	-4.85292900	-2.91929800	-0.00378300

DMMS

0 1

Si	-0.00049100	0.51088900	0.30636700
H	0.00012100	0.22274300	1.77512500
C	-0.00198100	2.32477000	-0.11744200
H	-0.89078100	2.82096100	0.28666600
H	0.88610800	2.82238000	0.28648900
H	-0.00219700	2.46359500	-1.20402500
O	1.39267100	-0.13087000	-0.32800900

O	-1.39301900	-0.13289900	-0.32737800
C	-1.92329400	-1.40566600	0.00102000
H	-2.99934500	-1.39466600	-0.20064900
H	-1.46530400	-2.19389800	-0.61144200
H	-1.77311800	-1.65455700	1.06173800
C	1.92614700	-1.40207300	0.00125800
H	1.47045200	-2.19180100	-0.61098700
H	3.00224600	-1.38839400	-0.20001500
H	1.77623800	-1.65084100	1.06204300

Intl'

0 1

C	0.64360700	0.31151100	0.77742100
C	-1.20670800	-0.80133600	-0.06555100
C	-0.43029800	1.18884200	0.64360000
N	0.09439800	-0.89847300	0.33542600
N	-1.55056700	0.50184900	0.10935300
C	-0.39699500	2.61439100	1.01555800
C	-1.51640700	3.40523500	1.33810100
C	0.87463300	3.22085400	1.10260700
C	-1.36835600	4.74253300	1.71357900
H	-2.51366000	2.98711800	1.30498200
C	1.01759000	4.55035400	1.48353500
H	1.74334500	2.61352900	0.87529300
C	-0.10497200	5.32615900	1.78749800
H	-2.25367200	5.32498200	1.95670400
H	2.01219300	4.98606700	1.53974600
H	0.00567100	6.36665500	2.08092900
C	-2.07510600	-1.89266800	-0.53718600
C	-2.04278600	-3.14447800	0.10766300
C	-2.94849600	-1.73235400	-1.62980900
C	-2.84806500	-4.19410700	-0.32830100
H	-1.38845100	-3.29499500	0.95695400
C	-3.75657900	-2.78381100	-2.05800200
H	-2.99687000	-0.78413500	-2.14855200
C	-3.71005700	-4.02050700	-1.41245900
H	-2.80457800	-5.14888800	0.18834100
H	-4.41963700	-2.63431700	-2.90567900
H	-4.33837100	-4.83978400	-1.75057800
C	0.91058200	-2.09143500	0.26727500
C	1.20122600	-2.77234500	1.46932700
C	1.44692300	-2.49002200	-0.97227500
C	2.04786300	-3.88386400	1.39686700
C	2.28102300	-3.61619700	-0.98600100
C	2.58175800	-4.30701000	0.18223100
H	2.29571200	-4.42548600	2.30478600
H	2.70979500	-3.94642000	-1.92790400

H	3.23765400	-5.17308100	0.14894500
C	-2.83606100	1.06094000	-0.24771600
C	-3.94080100	0.84251800	0.60355800
C	-2.93205800	1.83156800	-1.42808700
C	-5.16604700	1.41020300	0.23264600
C	-4.18368800	2.37297600	-1.74577700
C	-5.29126400	2.16589500	-0.92906400
H	-6.03405900	1.25982300	0.86812500
H	-4.28943300	2.96920600	-2.64759300
H	-6.25227500	2.59739600	-1.19615000
C	-1.74506800	2.10120200	-2.35410000
H	-0.86066500	1.62019300	-1.92692400
C	-3.84829800	0.04904600	1.90575400
H	-2.83755400	-0.36115500	1.98472600
C	0.64857700	-2.31849700	2.81951300
H	-0.19284500	-1.64413300	2.62817500
C	1.18093900	-1.74439700	-2.27728600
H	0.51686400	-0.90247800	-2.06036800
C	-4.06499900	0.95675800	3.13382700
H	-5.06466300	1.40725200	3.12701300
H	-3.96921400	0.37203400	4.05618100
H	-3.32913700	1.76631400	3.17048700
C	-4.83128900	-1.13780500	1.92553900
H	-4.68299300	-1.79747200	1.06551600
H	-4.68822300	-1.72851000	2.83785600
H	-5.87327400	-0.79684900	1.91559600
C	-1.43944100	3.60977600	-2.45371800
H	-0.54114500	3.77011800	-3.06109200
H	-2.26324500	4.15388500	-2.93134600
H	-1.26801900	4.04871900	-1.46735300
C	-1.96211300	1.50811200	-3.76113900
H	-1.08923500	1.71228000	-4.39190800
H	-2.10411000	0.42246100	-3.73302000
H	-2.83702400	1.94832700	-4.25378600
C	2.47750700	-1.15479700	-2.86569000
H	2.97245400	-0.47554700	-2.16565900
H	3.19236000	-1.94337800	-3.12913400
H	2.25332600	-0.59485500	-3.78205900
C	0.46950600	-2.64196700	-3.30933600
H	1.10247100	-3.48617400	-3.60748800
H	-0.46739000	-3.04733400	-2.91439800
H	0.23899900	-2.06812100	-4.21512500
C	1.70177400	-1.50335900	3.59604500
H	2.59847100	-2.10490700	3.79004100
H	1.98647900	-0.61785900	3.02184000
H	1.29620800	-1.17871300	4.56236300
C	0.11547500	-3.48435600	3.67300900
H	-0.62230700	-4.08832900	3.13128700

H	0.91761800	-4.15544800	4.00047500
H	-0.36681300	-3.09320300	4.57626800
Si	5.51200500	0.56820800	-0.01254600
O	7.00390900	1.19434700	0.38433000
O	4.93771800	1.20626600	-1.44236100
C	8.15884000	0.98116300	-0.41157700
H	8.12926900	1.58173400	-1.33048400
H	9.03695600	1.27886100	0.17085300
H	8.27139100	-0.07572400	-0.69343100
C	4.50100700	2.54935100	-1.58573900
H	5.29357400	3.26558000	-1.32925200
H	4.22015700	2.70543800	-2.63229500
H	3.62396400	2.75699700	-0.95810900
C	4.39238100	0.91797300	1.43622500
H	3.34760100	0.66321600	1.20997900
H	4.70742100	0.33300000	2.30843500
H	4.43586200	1.97579100	1.72236600
H	5.66360600	-0.87543300	-0.33352700

TS1'

0 1

C	0.47131800	0.51902400	1.04274000
C	1.87907600	0.24625100	-0.71945800
C	0.95625900	-0.76578700	1.06812100
N	1.06427000	1.12676000	-0.07249800
N	1.81090200	-0.92756400	-0.03461100
C	0.71834700	-1.83348600	2.07209200
C	1.64885000	-2.03425600	3.10292500
C	-0.45234900	-2.60557800	2.04420700
C	1.43429400	-3.01634500	4.06834700
H	2.52347200	-1.39532900	3.16244000
C	-0.66360800	-3.58680800	3.01546400
H	-1.20769400	-2.41690000	1.28516000
C	0.27994700	-3.80104200	4.02063500
H	2.16074800	-3.15926300	4.86373000
H	-1.57556200	-4.17665500	2.98724400
H	0.10987000	-4.56543100	4.77426000
C	2.71330600	0.51564900	-1.91207800
C	3.29680600	1.78092100	-2.12076100
C	2.96303100	-0.48710500	-2.86912900
C	4.09493000	2.02756900	-3.23527700
H	3.13020700	2.58235400	-1.41824600
C	3.75861700	-0.23299800	-3.98388000
H	2.53346500	-1.46991000	-2.75639400
C	4.33103900	1.02417400	-4.17475400
H	4.53192800	3.01354400	-3.36387400
H	3.92321100	-1.02666400	-4.70672400

H	4.95073000	1.22013600	-5.04514500
C	0.82807400	2.50384100	-0.49412500
C	1.47148800	3.54503700	0.21636700
C	0.00005200	2.73740800	-1.61386000
C	1.29396400	4.84706600	-0.26549400
C	-0.13882700	4.06694600	-2.03701100
C	0.50542000	5.10905400	-1.38214400
H	1.77966900	5.67056200	0.24829200
H	-0.76596000	4.28025100	-2.89707700
H	0.38589900	6.13011800	-1.73492100
C	2.52060300	-2.15920300	-0.36203800
C	3.88366400	-2.26750800	-0.01482100
C	1.81917400	-3.18862800	-1.03460400
C	4.55575100	-3.43327100	-0.40383300
C	2.55035400	-4.32705700	-1.39479800
C	3.90336200	-4.44843800	-1.09410600
H	5.60770300	-3.54435300	-0.15857700
H	2.04424400	-5.13088300	-1.91994000
H	4.44765200	-5.34150100	-1.38932300
C	0.33618500	-3.11030000	-1.39066800
H	-0.09120600	-2.27409800	-0.83594200
C	4.65533100	-1.19562800	0.75281900
H	3.95316000	-0.40905100	1.04945300
C	2.35306900	3.33162000	1.45155800
H	2.18885400	2.32081500	1.83080000
C	-0.73420500	1.64570000	-2.39048700
H	-0.58013100	0.69069600	-1.88133400
C	5.27911300	-1.76436700	2.04411400
H	6.07574600	-2.48292900	1.82060500
H	5.72320800	-0.95514900	2.63518800
H	4.53546200	-2.27549200	2.66217800
C	5.75049800	-0.54347100	-0.11608900
H	5.34098000	-0.10397800	-1.02933200
H	6.25708700	0.24845600	0.44799800
H	6.50864400	-1.27963900	-0.40796000
C	-0.43941600	-4.37009400	-0.95941000
H	-1.51016600	-4.18954600	-1.09905300
H	-0.16789800	-5.23947400	-1.56983400
H	-0.25921300	-4.62020500	0.09022500
C	0.06682600	-2.83807700	-2.88635500
H	-1.00984000	-2.68803900	-3.02483000
H	0.57013700	-1.93468100	-3.24515600
H	0.39998300	-3.67933000	-3.50703100
C	-2.25706600	1.88348000	-2.42471800
H	-2.66426000	1.99616900	-1.41734600
H	-2.50901300	2.77793600	-3.00767400
H	-2.74597600	1.02189100	-2.89038600
C	-0.19871200	1.51094800	-3.83166600

H	-0.40133100	2.41926600	-4.41197400
H	0.87917900	1.32917200	-3.86254700
H	-0.70306800	0.67756800	-4.33295800
C	1.96699800	4.28841900	2.59671900
H	2.23446500	5.32728900	2.36856600
H	0.89549900	4.23557500	2.79880200
H	2.50727200	4.00460500	3.50670000
C	3.85624600	3.48017900	1.13304500
H	4.21543000	2.72243700	0.42898200
H	4.07713800	4.46658900	0.70708300
H	4.44232200	3.37763900	2.05381100
Si	-0.70749900	1.29128000	2.35826300
H	-1.97643200	1.11671600	0.68895200
H	-2.27472900	0.34993900	0.30191100
N	-2.48556000	-0.93713200	-0.30629200
H	-1.58873500	-1.13923000	-0.74966600
C	-3.42816100	-1.24642500	-1.22446900
C	-4.85541200	-0.94303400	-0.84494400
C	-5.22505200	-0.43363000	0.41043200
C	-5.86326600	-1.17939400	-1.78342500
C	-6.55453800	-0.16595000	0.71095000
H	-4.45856000	-0.25121000	1.15571300
C	-7.20427700	-0.91677500	-1.49914500
H	-5.56939400	-1.57803800	-2.74910800
C	-7.55397000	-0.40600000	-0.24341100
H	-6.84844800	0.22595800	1.68043600
H	-7.95892800	-1.11188100	-2.25336500
O	-3.19811200	-1.75866300	-2.34516900
O	-8.83307200	-0.11102500	0.14904000
C	-9.88233900	-0.34120800	-0.77341700
H	-10.80205900	-0.04578100	-0.26371600
H	-9.76376800	0.26273200	-1.68348100
H	-9.95019600	-1.40063200	-1.05614800
O	0.51556200	1.38643700	3.52675200
O	-1.07343400	2.90841200	2.20123400
C	0.27381500	1.86492200	4.83614500
H	1.20681800	1.79788800	5.40750300
H	-0.05673900	2.91202900	4.83136800
H	-0.48693100	1.26543700	5.35805500
C	-2.21232300	3.51912100	1.61709700
H	-3.13516600	2.97258500	1.84332000
H	-2.28915000	4.53190600	2.02808800
H	-2.10789800	3.58121200	0.52909200
C	-2.04931600	0.20365700	3.10389400
H	-2.40761000	-0.54644400	2.39613100
H	-1.69708100	-0.30128200	4.01001900
H	-2.90466400	0.83513000	3.37646600

DMMSO

-1 1

Si	-0.00006300	0.41195600	0.20842800
C	0.00020200	2.23094800	-0.34097200
H	-0.88712000	2.75419600	0.03717000
H	0.88796100	2.75375600	0.03675500
H	-0.00003000	2.31560600	-1.43565400
O	1.36153500	-0.16537200	-0.66996900
O	-1.36269900	-0.16437900	-0.66896500
C	-2.08643600	-1.26404800	-0.18706500
H	-3.16067300	-1.13073200	-0.40610200
H	-1.77401500	-2.20818300	-0.67351100
H	-1.96169800	-1.38703900	0.89783400
C	2.08678900	-1.26362900	-0.18711700
H	1.77572700	-2.20855200	-0.67290500
H	3.16088300	-1.12902600	-0.40612200
H	1.96206500	-1.38592900	0.89785400
O	0.00047100	0.03461300	1.72613500

DMMSOH

0 1

Si	-0.00056100	0.47403600	0.02557500
C	-0.00242000	2.25499400	-0.51845200
H	-0.89256300	2.78445700	-0.16177000
H	0.88705000	2.78602900	-0.16243900
H	-0.00289900	2.30804200	-1.61244100
O	1.37376600	-0.21895000	-0.57627700
O	-1.37443700	-0.22100900	-0.57502800
C	-1.95681600	-1.43846400	-0.13409900
H	-2.98769300	-1.47485200	-0.50049200
H	-1.41645500	-2.30487100	-0.53875000
H	-1.96742700	-1.50688900	0.96056200
C	1.96007200	-1.43414400	-0.13430600
H	1.42168200	-2.30262600	-0.53713100
H	2.99062300	-1.46815200	-0.50184600
H	1.97212800	-1.50100600	0.96042900
O	0.00074700	0.27270000	1.68316800
H	-0.00221800	1.08711900	2.20206500

DMMS2O

0 1

Si	1.64382100	-0.42367600	-0.23356900
C	1.68139200	-2.06316000	-1.11296800
H	0.83252900	-2.68518200	-0.80932800
H	1.61783100	-1.91715600	-2.19681200

H	2.60789800	-2.60519300	-0.89709100
O	2.87840500	0.49011100	-0.82395000
O	1.88054400	-0.54315100	1.40069800
C	0.93319100	-1.02103400	2.34462600
H	0.63802300	-2.05753300	2.13234300
H	1.39968900	-0.99106800	3.33437500
H	0.03018000	-0.39833400	2.36062200
C	3.18695000	1.80162000	-0.37301200
H	3.40540400	1.81163800	0.70165500
H	4.07183800	2.14571800	-0.91705900
H	2.35971600	2.49476700	-0.57487400
O	0.21018500	0.36352600	-0.52254100
Si	-1.42278200	0.25516200	-0.42501800
C	-2.17492100	1.03953300	-1.94418000
H	-3.26706900	0.94789100	-1.94470900
H	-1.92941100	2.10579100	-2.00907200
H	-1.79347000	0.55802600	-2.85110000
O	-1.98409800	0.96747500	0.96510300
O	-1.79458500	-1.34947300	-0.28308900
C	-1.76891200	2.32736300	1.31281800
H	-2.19914200	3.01002100	0.56703300
H	-2.25900100	2.51483300	2.27301400
H	-0.69889100	2.54822000	1.41603500
C	-3.06427100	-1.84645200	0.11875400
H	-3.35655300	-1.44644800	1.09658900
H	-3.84403800	-1.59563700	-0.61351200
H	-2.99425200	-2.93630100	0.18611900

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