

## Selective Catalytic Hydrogenation of Nitriles to Primary Amines Using Iron Pincer Complexes

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### FeBr<sub>2</sub>·2THF:

FeBr<sub>2</sub> was placed into a flamed dried Soxhlett (30 mL extraction volume) and extracted over a period of 4 hours (until the extract is colourless). The orange-brownish extract was cooled down to room temperature to give off white flaky crystals in a dark brown mother-liquor. The liquid was removed while the product is cooled down to -78°C. The solid was recrystallized 3-4 times and washed with small portions of cold dry THF until the liquid becomes nearly colorless. After vacuum-drying the off-white product (80% yields) should be stored in a freezer.

### Synthesis of [FeBr<sub>2</sub>(CO)(HN(CH<sub>2</sub>CH<sub>2</sub>PCy<sub>2</sub>)<sub>2</sub>)]:

The ligand HN(CH<sub>2</sub>CH<sub>2</sub>PCy<sub>2</sub>)<sub>2</sub> (1.21 g, 2.61 mmol) was dissolved in 25 mL THF (abs.) at room temperature in a 100 mL Schlenk tube under argon. 932.7 mg FeBr<sub>2</sub>·2THF (2.61 mmol) in 20 mL ethanol was added dropwise over a period of 5-10 minutes. A white fluffy precipitate was formed and the mixture was stirred over night at room temperature. CO was bubbled through the suspension for 1 hour until the precipitate is dissolved completely and the solution turned to dark blue. After removing the CO by bubbling Argon through the solution the solvents were removed under reduced pressure to obtain a blue crystalline solid. The product was washed 3 times with 10 mL ethanol and dried under vacuum.

Yield: 1.78 g (2.5 mmol, 96 %).

**<sup>1</sup>H NMR** (400 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 5.39 (t, *J* = 12.8 Hz, 1H, NH), 3.76 – 3.60 (m, 2H, CH<sub>2</sub>), 3.51 – 3.26 (m, 2H, CH<sub>2</sub>), 2.59 – 2.32 (m, 6H), 2.20 (dd, *J* = 22.5, 12.6 Hz, 4H), 2.08 – 1.57 (m, 26H), 1.38 – 1.04 (m, 13H).

**<sup>31</sup>P NMR** (162 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 59.92.

**<sup>13</sup>C NMR** (101 MHz, CD<sub>2</sub>Cl<sub>2</sub>): δ 227.50 (s, CO), 50.66 (s, CH<sub>2</sub>), 36.34 (t, *J*<sub>CP</sub> = 10.4 Hz, CH), 34.66 (t, *J*<sub>CP</sub> = 8.9 Hz, CH), 30.72 (s), 29.94 (s), 29.27 (s), 28.72 – 27.49 (m), 26.94 (d, *J*<sub>CP</sub> = 12.2 Hz), 24.84 (t, *J*<sub>CP</sub> = 7.3 Hz).

**IR** (ATR): 3229,9 cm<sup>-1</sup> (NH), 3177.4 cm<sup>-1</sup> (NH), 2918.1 cm<sup>-1</sup>, (CH<sub>2</sub>), 2845,3 cm<sup>-1</sup> (CH<sub>2</sub>), 1942.7 cm<sup>-1</sup> (CO) cm<sup>-1</sup>.

**HRMS**: calc. for C<sub>28</sub> H<sub>53</sub> Br Fe N P<sub>2</sub> 602.21648, found 602.21635 (Fe –HBr –CO).

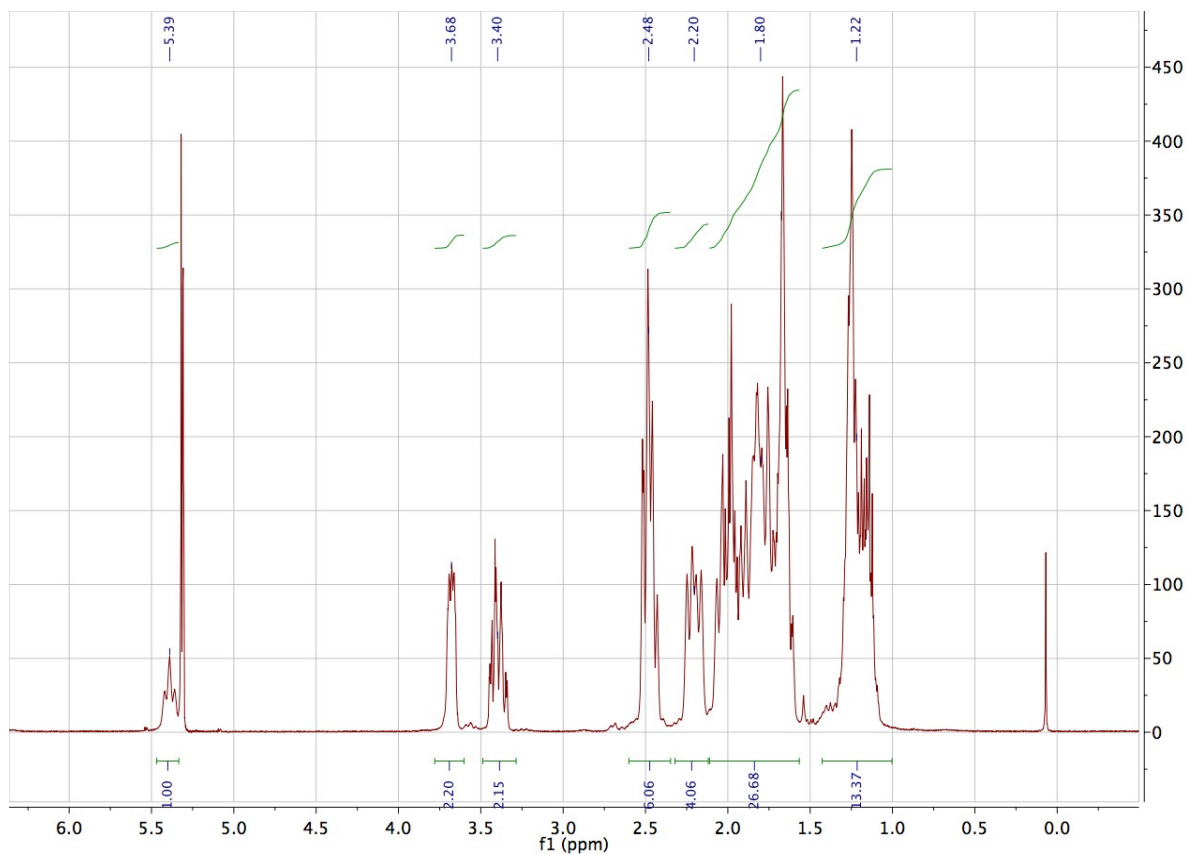


Figure SI 1:  $^1\text{H}$  NMR of compound 4  $\text{CD}_2\text{Cl}_2$ .

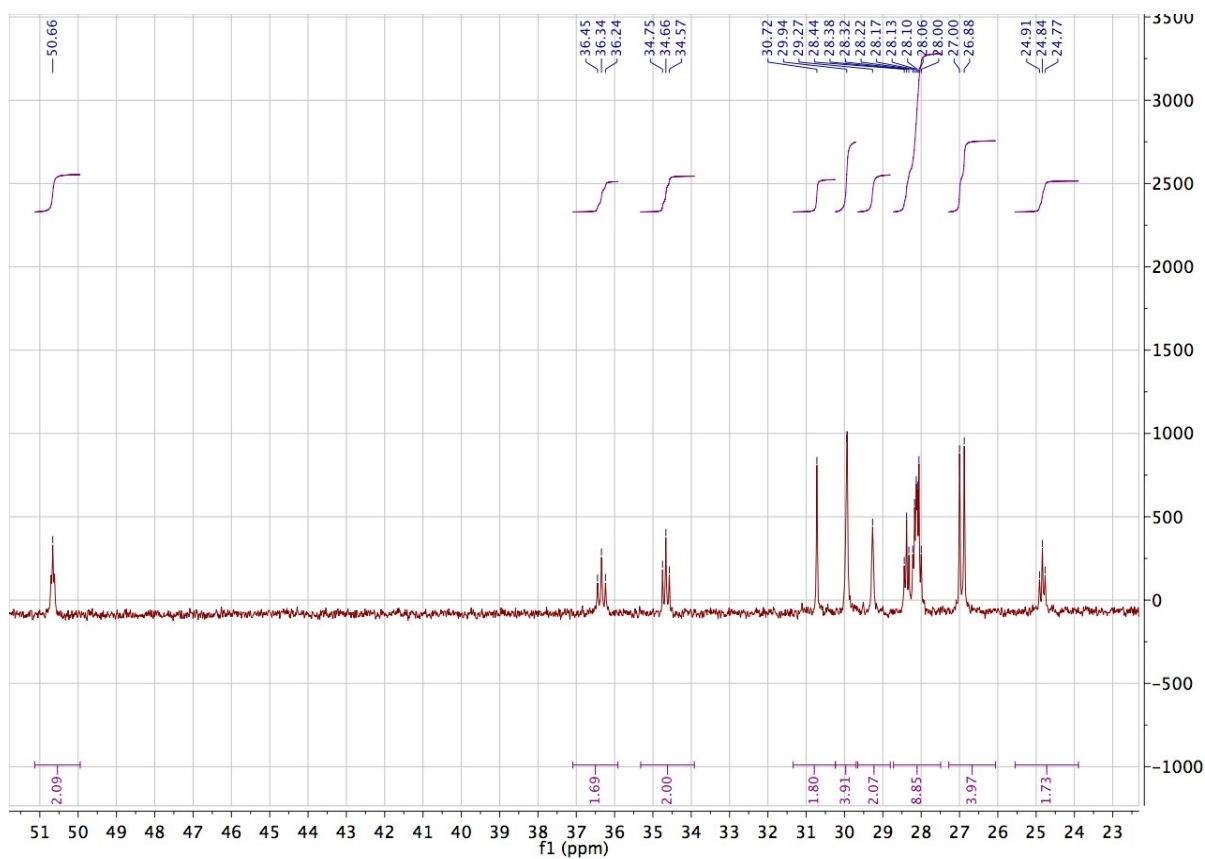


Figure SI 2:  $^{13}\text{C}$  NMR of compound 4 in  $\text{CD}_2\text{Cl}_2$ .

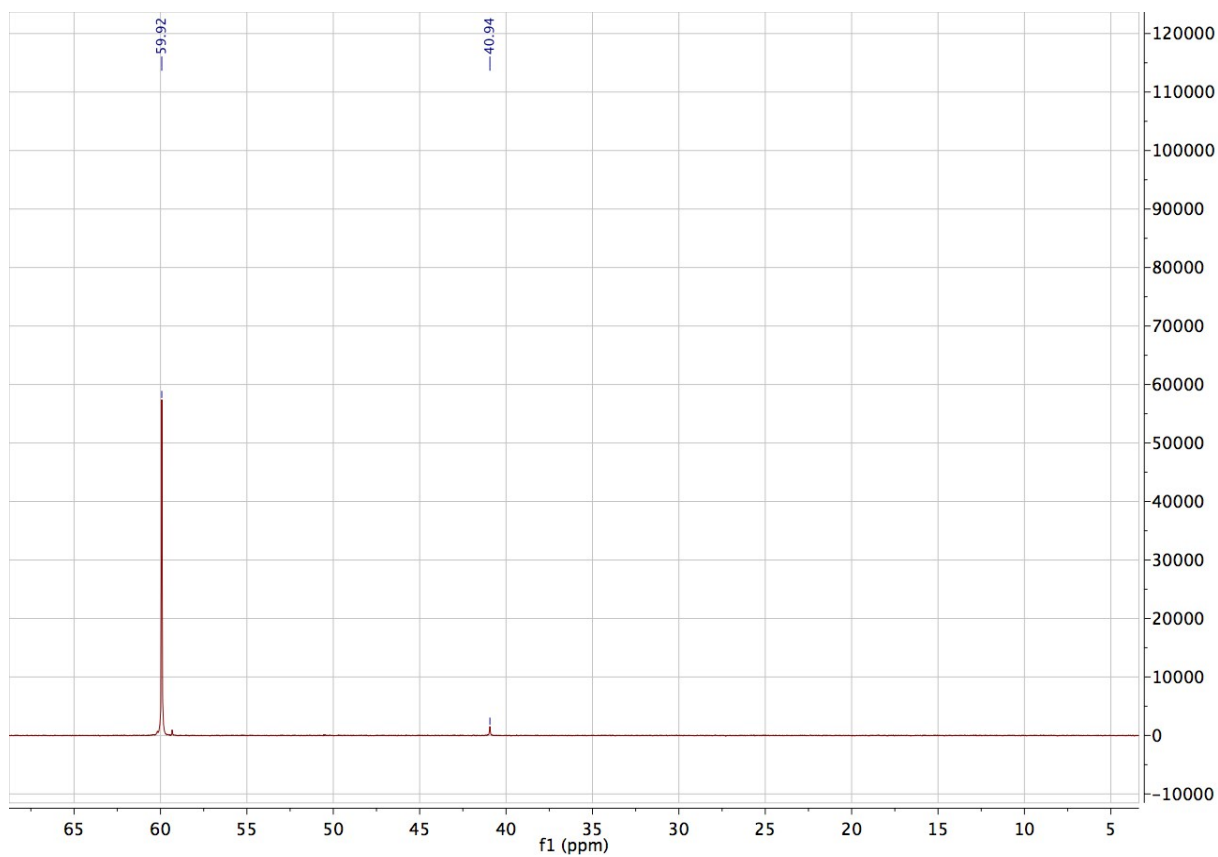


Figure SI 3:  $^{31}\text{P}$  NMR of compound **4** in  $\text{CD}_2\text{Cl}_2$ .

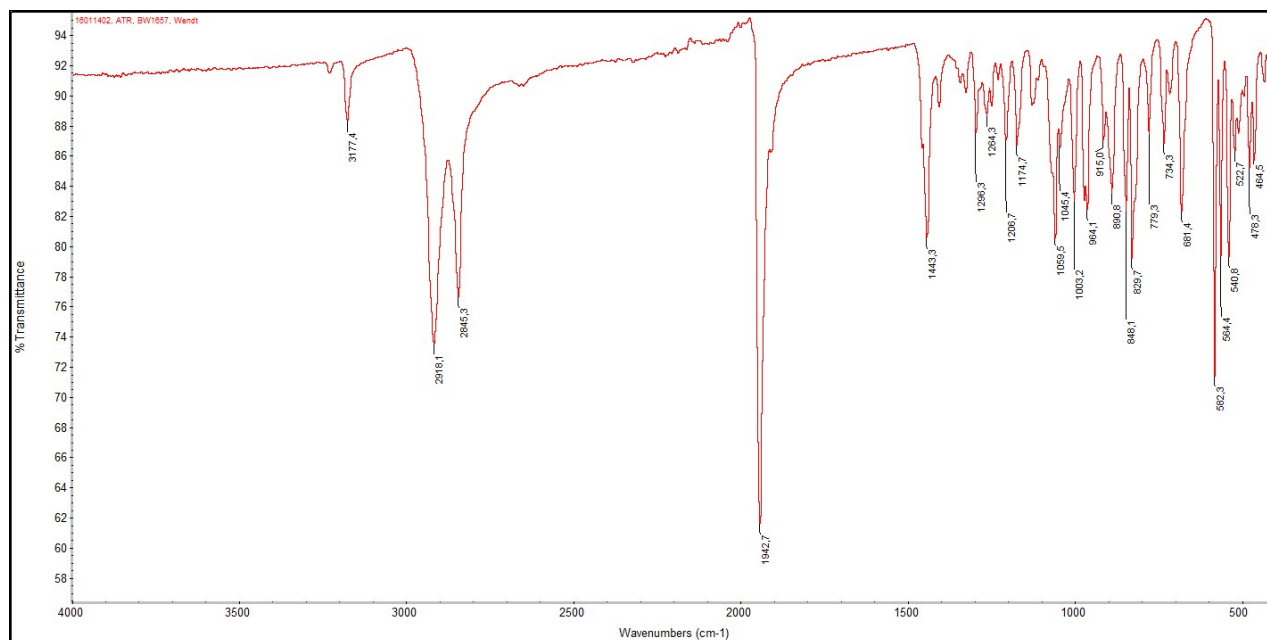


Figure SI 4: IR ATR spectra of **4**.

### Synthesis of [Fe(CO)(H)(HBH<sub>3</sub>)(HN(CH<sub>2</sub>CH<sub>2</sub>PCy<sub>2</sub>)<sub>2</sub>)] 2:

254.1 mg (0.36 mmol) of [FeBr<sub>2</sub>(CO)(HN(C<sub>2</sub>H<sub>4</sub>PCy<sub>2</sub>)<sub>2</sub>)] were placed in an evacuated 50 mL Schlenk-tube under argon and 10 mL of dry ethanol were added. NaBH<sub>4</sub> (136.2 mg, 3.6 mmol, 10 eq.) was gradually added to the suspension. During 2 hours of stirring at room temperature the color of the solution changed from blue, to green and finally to yellow. The solvent was evaporated under vacuum. The yellow solid was dissolved in toluene to give a bright yellow solution with white precipitate. After the solution was filtered, the toluene was evaporated under vacuum. The yellow solid was recrystallized from a mixture of THF and n-heptane and washed 5 times with 10 mL of n-heptane. The product was obtained as a yellow powder. Yield: 154.7 mg (0.27 mmol, 76 %)

**<sup>1</sup>H NMR** (300 MHz, Benzene-*d*<sub>6</sub>) δ 3.97 (br, 1H, NH), 2.88 (d, *J*<sub>HP</sub> = 11.7 Hz, 2H), 2.54 (m, 4H), 2.22 – 2.02 (m, 2H), 2.00 – 1.44 (m, 27H), 1.44 – 1.02 (m, 14H), 0.95 – 0.84 (m, 2H), -2.79 (br, 4H, BH<sub>4</sub>), major isomer δ -19.57 (t, *J*<sub>HP</sub> = 52 Hz, 1H, FeH, 72 %), minor isomer δ -20.44 (t, *J* = 52.1 Hz, 1H, FeH, 28%).

**<sup>31</sup>P NMR** (122 MHz, C<sub>6</sub>D<sub>6</sub>, 298 K) minor isomer δ = 92.70 (d, *J* = 5 Hz, 31%), major isomer δ 91.54 (d, *J* = 11.2 Hz, 69 %), impurities 47.47.

**<sup>13</sup>C NMR** (101 MHz, Benzene-*d*<sub>6</sub>): δ 54.17 (t, *J*<sub>CP</sub> = 5.6 Hz, CH<sub>2</sub>), 40.10 (t, *J*<sub>CP</sub> = 9.3 Hz, CH), 36.60 (t, *J*<sub>CP</sub> = 12.6 Hz, CH), 32.11 (s), 31.32 (s), 30.31 (s), 29.12 (t, *J*<sub>CP</sub> = 52.0 Hz), 28.26 (s), 28.20 (s), 28.05 (s), 27.96 (s), 27.85 (t, *J*<sub>CP</sub> = 4.3 Hz), 27.39 (t, *J*<sub>CP</sub> = 4.6 Hz), 27.17 (t, *J*<sub>CP</sub> = 6.3 Hz), 26.83 (s), 26.69 (s), 23.12 (s), 14.38 (s), CO not observed.

**IR** (ATR): 3198.0 cm<sup>-1</sup> (NH), 2917.9 cm<sup>-1</sup> (CH<sub>2</sub>), 2847.3 cm<sup>-1</sup> (CH<sub>2</sub>), 2360.3 cm<sup>-1</sup> (BH<sub>3</sub>), 1905.0 cm<sup>-1</sup> (CO).

**HRMS**: calc. for C<sub>29</sub>H<sub>57</sub>BFeNOP<sub>2</sub> 564.33581, found 564.33648 (Fe – H).

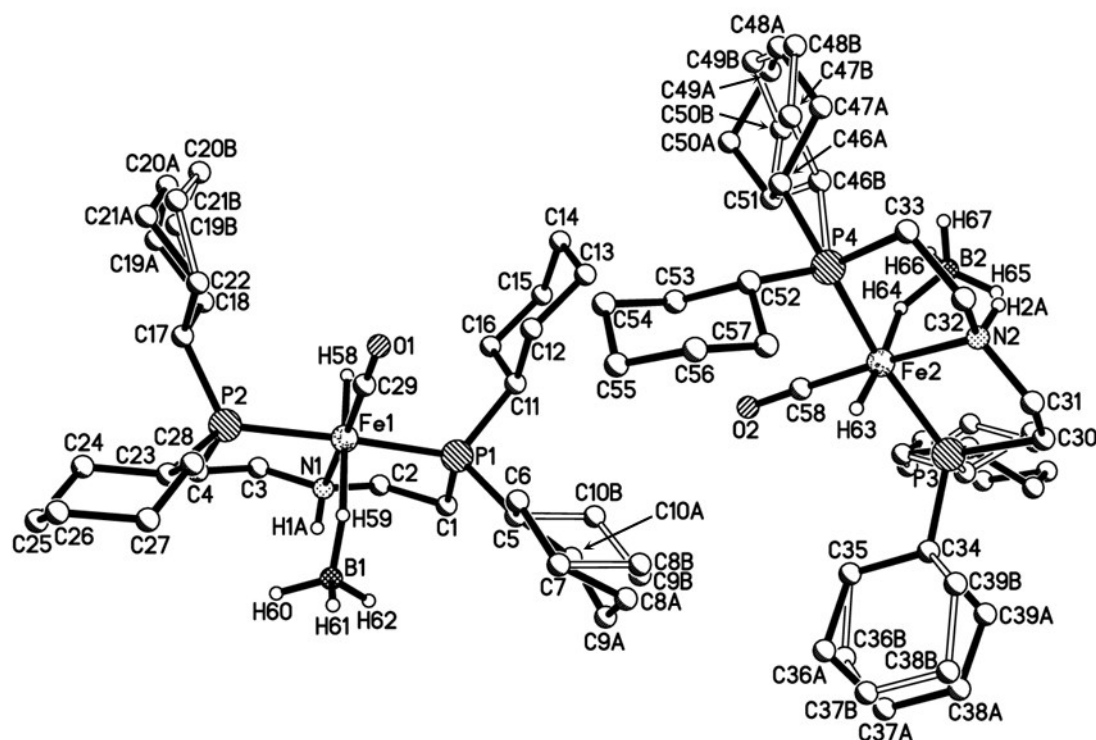
### X-ray crystal structure analysis of 2:

Data were collected on a Bruker Kappa APEX II Duo diffractometer. The structure was solved by direct methods and refined by full-matrix least-squares procedures on *F*<sup>2</sup> with the SHELXTL software package (G. M. Sheldrick, *Acta Crystallogr.* 2008, *A64*, 112–122.).

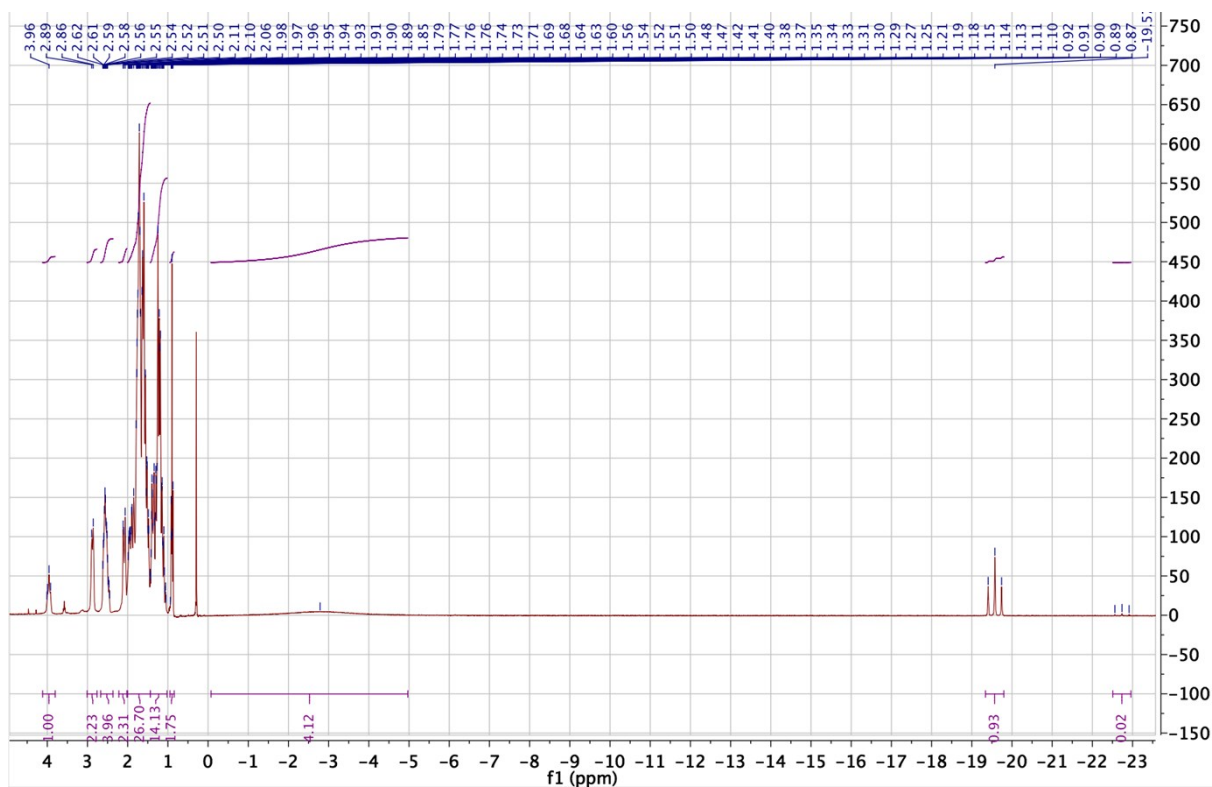
**Crystal data for complex 2:** C<sub>29</sub>H<sub>58</sub>BFeNOP<sub>2</sub>, *M* = 565.36, monoclinic, space group *P*2<sub>1</sub>/*n*, *a* = 16.4846(6), *b* = 24.0911(9), *c* = 17.4970(6) Å, β = 113.6636(16)°, *V* = 6364.4(4) Å<sup>3</sup>, *T* = 150(2) K, *Z* = 8, 45206 reflections measured, 8854 independent reflections (*R*<sub>int</sub> = 0.0375), final *R* values (*I* > 2σ(*I*)): *R*<sub>1</sub> = 0.0612, *wR*<sub>2</sub> = 0.1588, final *R* values (all data): *R*<sub>1</sub> = 0.0689, *wR*<sub>2</sub> = 0.1665, GOF on *F*<sup>2</sup>: 1.061, 645 parameters.

The structure of **2** is strongly disordered. A disorder of the cyclohexyl ring C52-C57 and in the backbone of the ligand in the second molecule of the asymmetric unit (see ADP of e.g. C31,

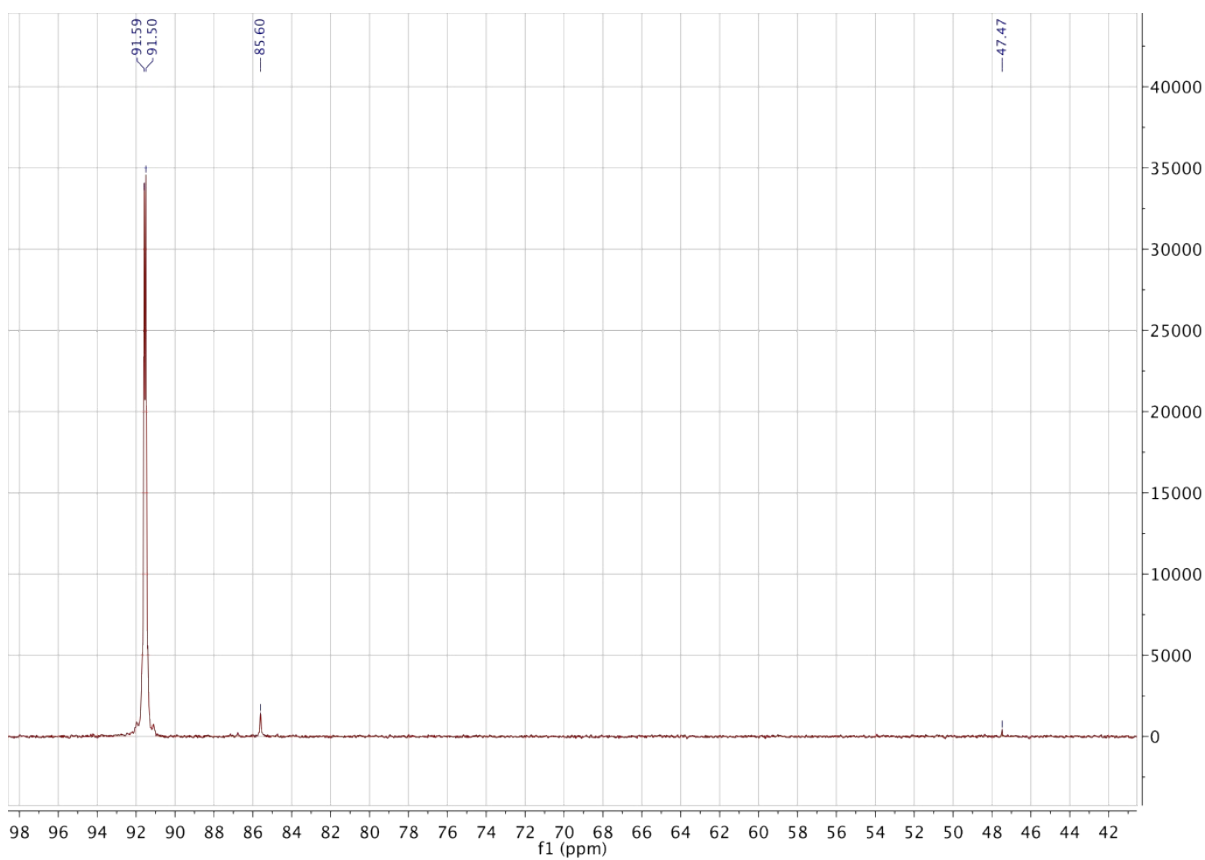
C32, C33) was not resolved. DFIX, SADI instructions were used to improve the geometry of the disordered parts of the molecules. Additionally, the isotropic displacement parameters of several C atoms (C39A and C39B; C40A, C42A, C43A, C44A, C45A and C40B, C42B, C43B, C44B, C45B; C46A-C50A and C46B-C50B) were restrained to be equal (EADP). H1A, H2A, H58-H67 could be found from the difference Fourier map and were refined freely.



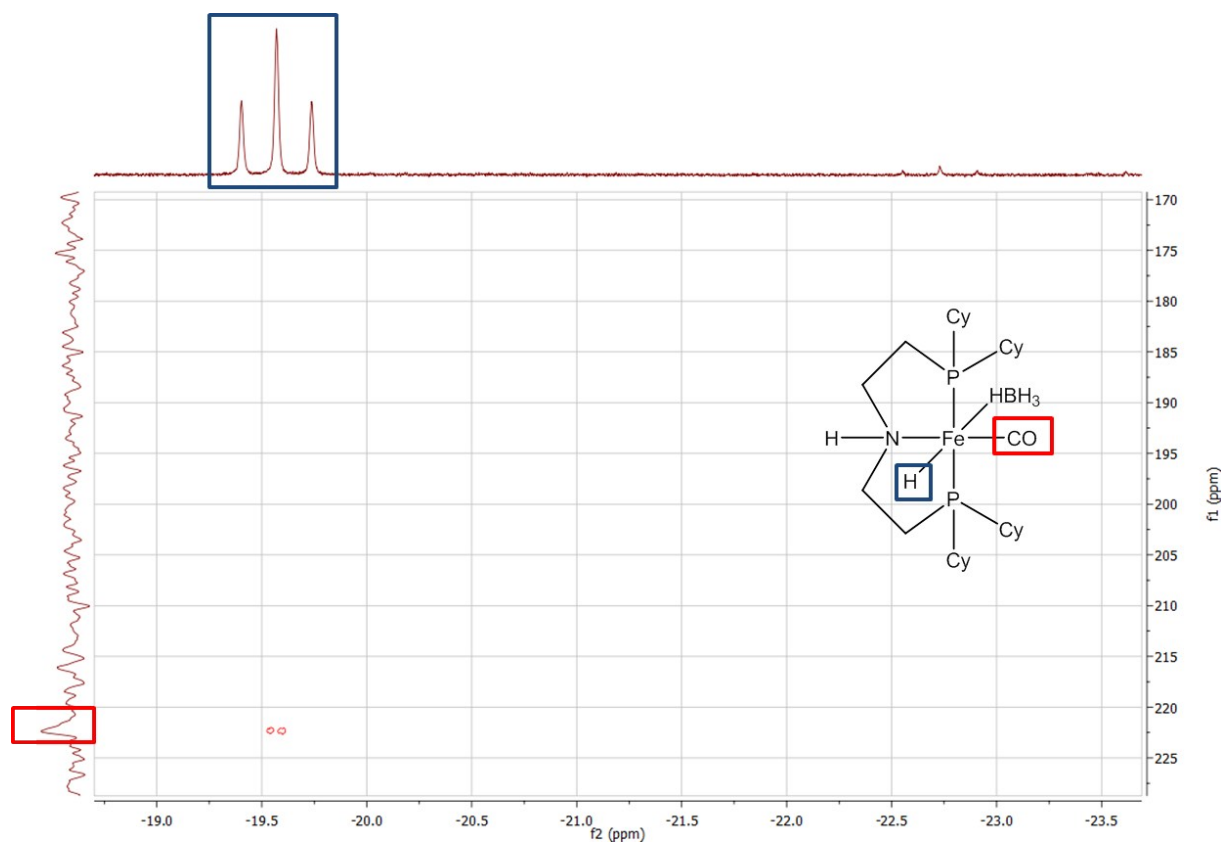
**Figure SI 5:** Ball-and-stick plot of **2** showing the numbering scheme (C41, C40A, C42A, C43A, C44A, C45A, C40B, C42B, C43B, C44B, C45B are not labelled). Hydrogen atoms (except H1A, H2A, H58-H67) are omitted for clarity. Selected bond lengths [Å] and angles [deg]: Fe1-N1 2.070(4), Fe1-P1 2.2171(12), Fe1-P2 2.2185(13), Fe1-H58 1.39(5), Fe1-H59 1.70(4), Fe1-C29 1.725(4), C29-O1 1.163(5), B1-H59 1.18(4), Fe2-N2 2.079(4), Fe2-P3 2.214(2), Fe2-P4 2.213(2), Fe2-H63 1.39(5), Fe2-H64 1.66(4), Fe2-C58 1.728(5), C58-O2 1.156(6), B2-H64 1.20(4); P1-Fe1-P2 168.49(5), N1-Fe1-P1 84.51(12), N1-Fe1-P2 84.45(12), C29-Fe1-N1 173.5(2), C29-Fe1-P1 94.88(14), C29-Fe1-P2 95.71(14), P3-Fe2-P4 167.96(6), N2-Fe2-P3 84.40(16), N2-Fe2-P4 84.18 (16), C58-Fe2-N2 173.1(2), C58-Fe2-P3 95.61(16) C58-Fe2-P4 95.27(16).



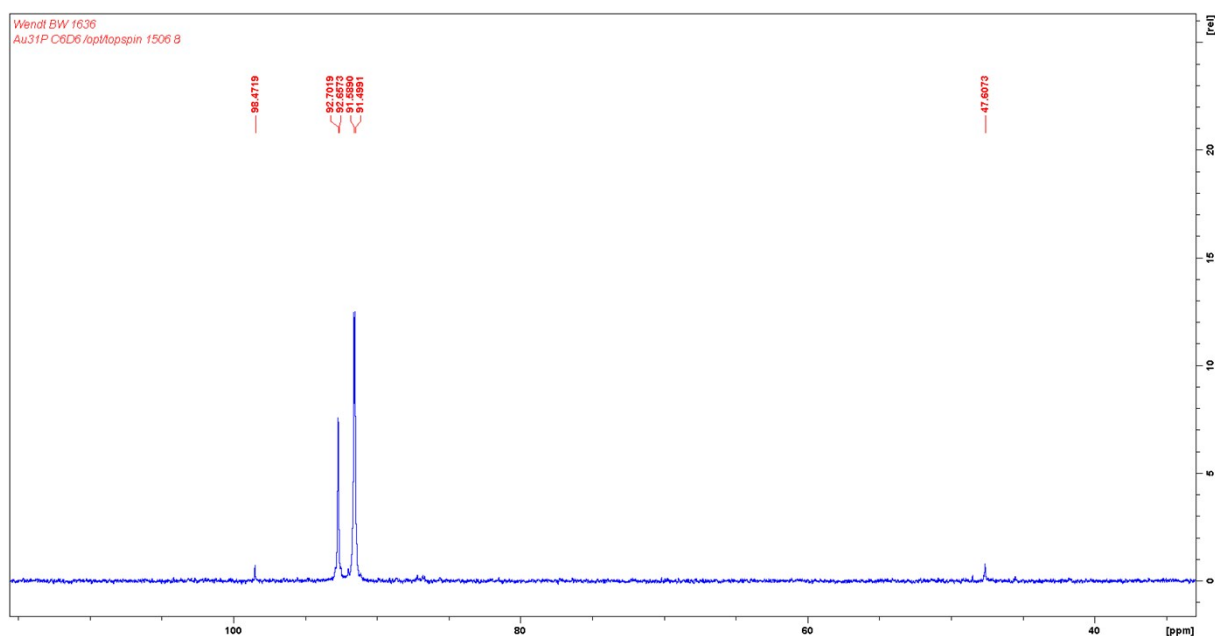
**Figure SI 6:**  $^1\text{H}$  NMR of compound **2** in  $\text{C}_6\text{D}_6$ .



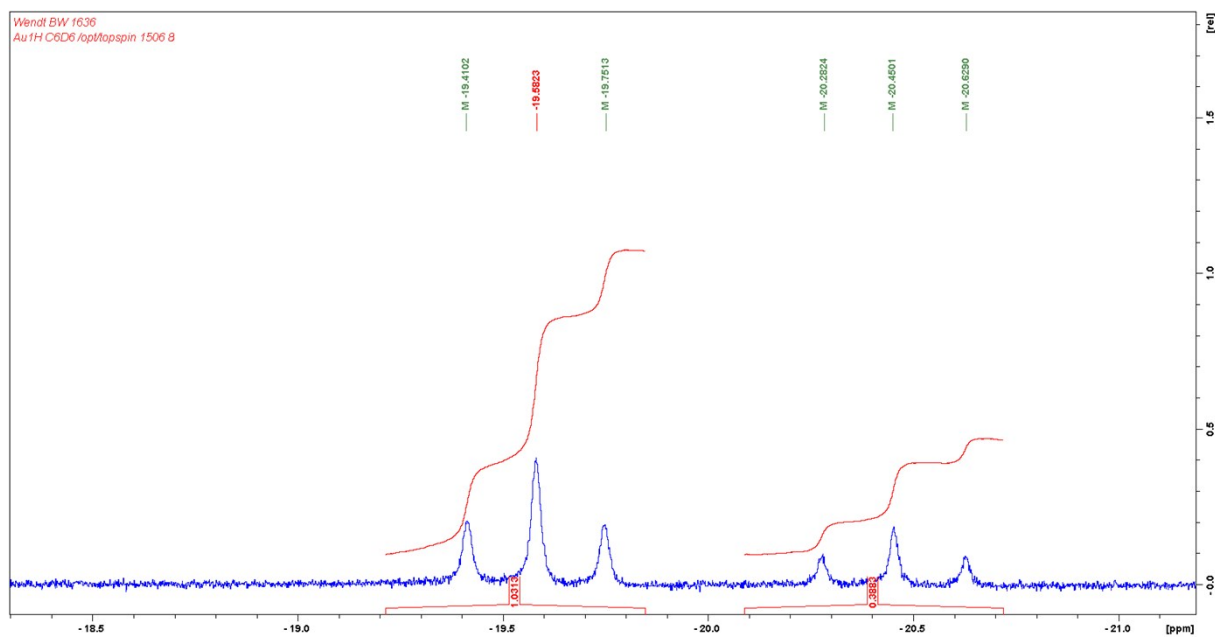
**Figure SI 7:**  $^{31}\text{P}$  NMR of compound **2** in  $\text{C}_6\text{D}_6$ . Major isomer is formed after keeping the sample for several hours at room temperature.



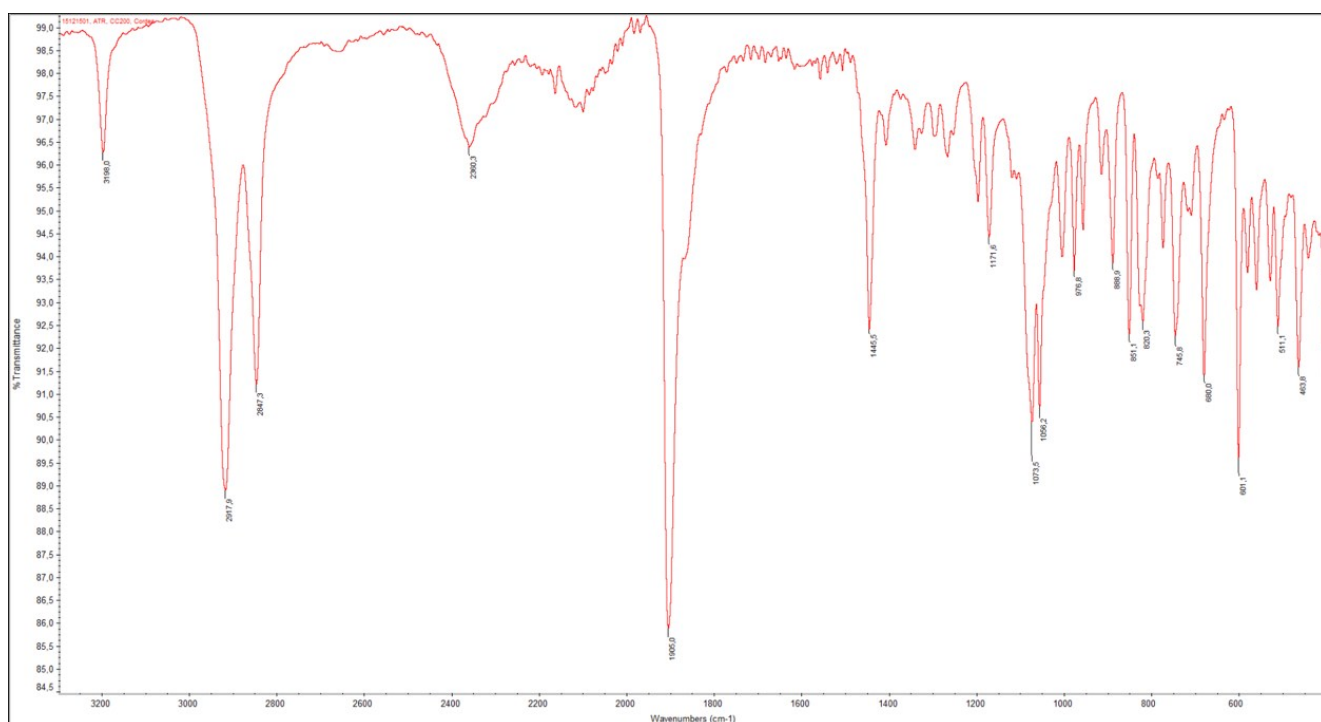
**Figure SI 8:**  $^1\text{H}$ - $^{13}\text{C}$  HMBC NMR of **2** (carbonyl region) in  $\text{C}_6\text{D}_6$ , representing the cross peak for the major isomer. CO signal for minor isomer not detectable due to low intensity.



**Figure SI 9:**  $^{31}\text{P}$  NMR of fresh prepared complex **2** in  $\text{C}_6\text{D}_6$  showing both isomers.



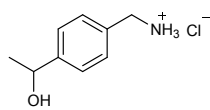
**Figure SI 10:**  $^1\text{H}$  NMR of fresh prepared complex **2** in  $\text{C}_6\text{D}_6$  showing the hydride signals of both isomers.



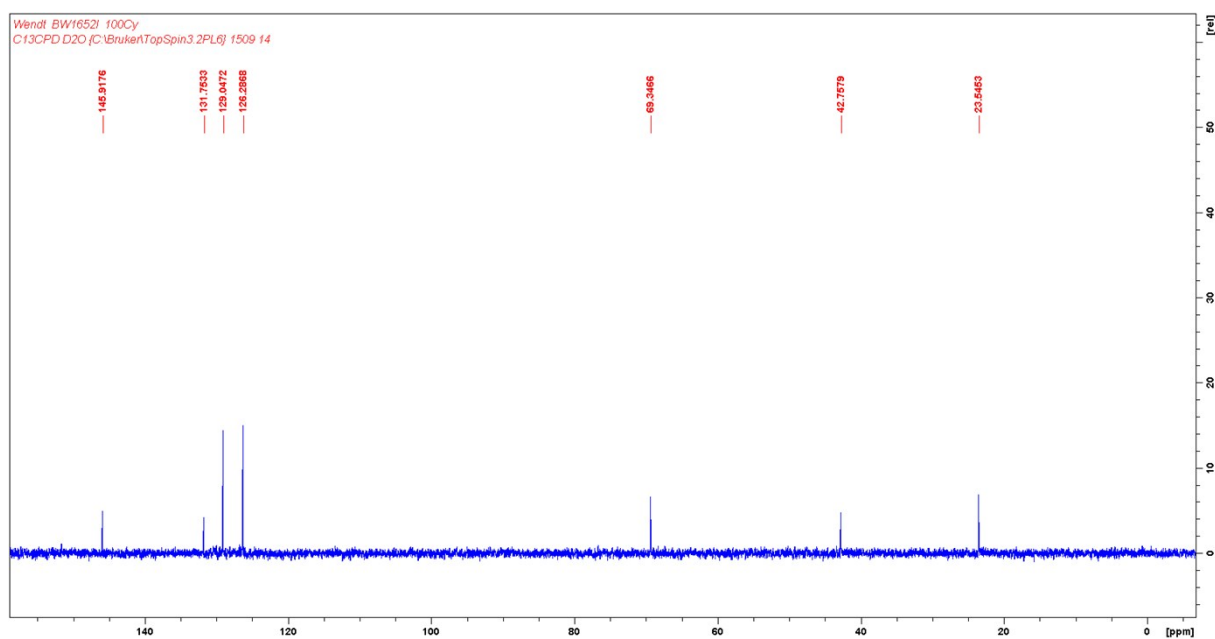
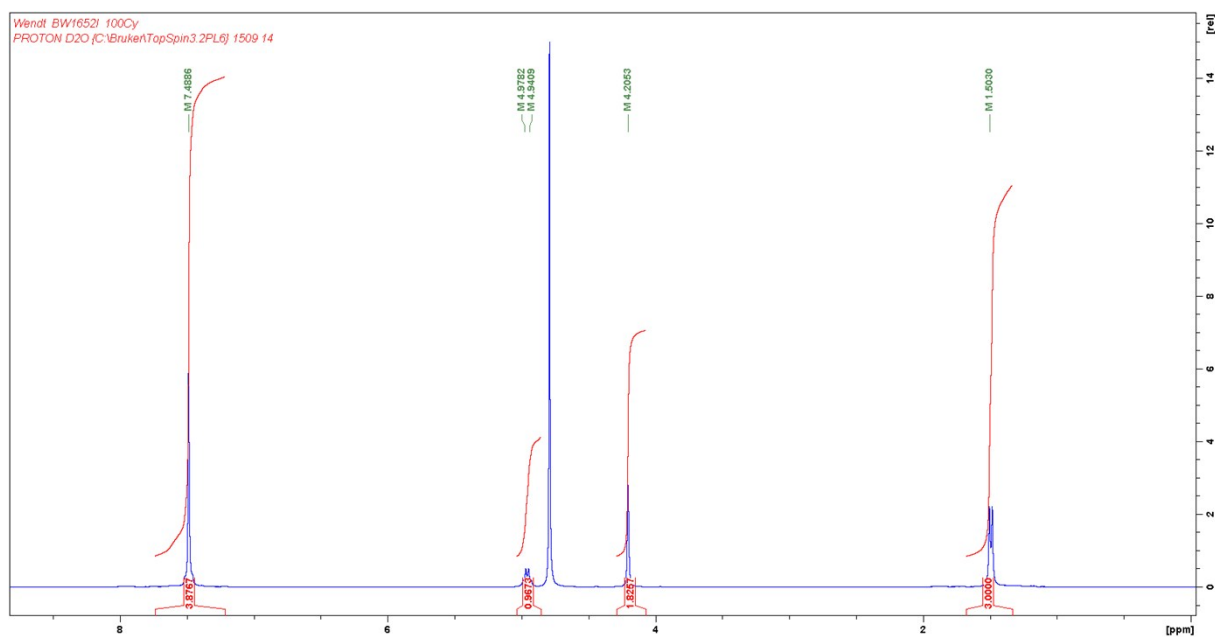
**Figure SI 11:** IR-ATR of compound **2**.

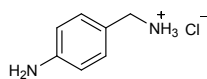


## Analysis of $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of isolated compounds:

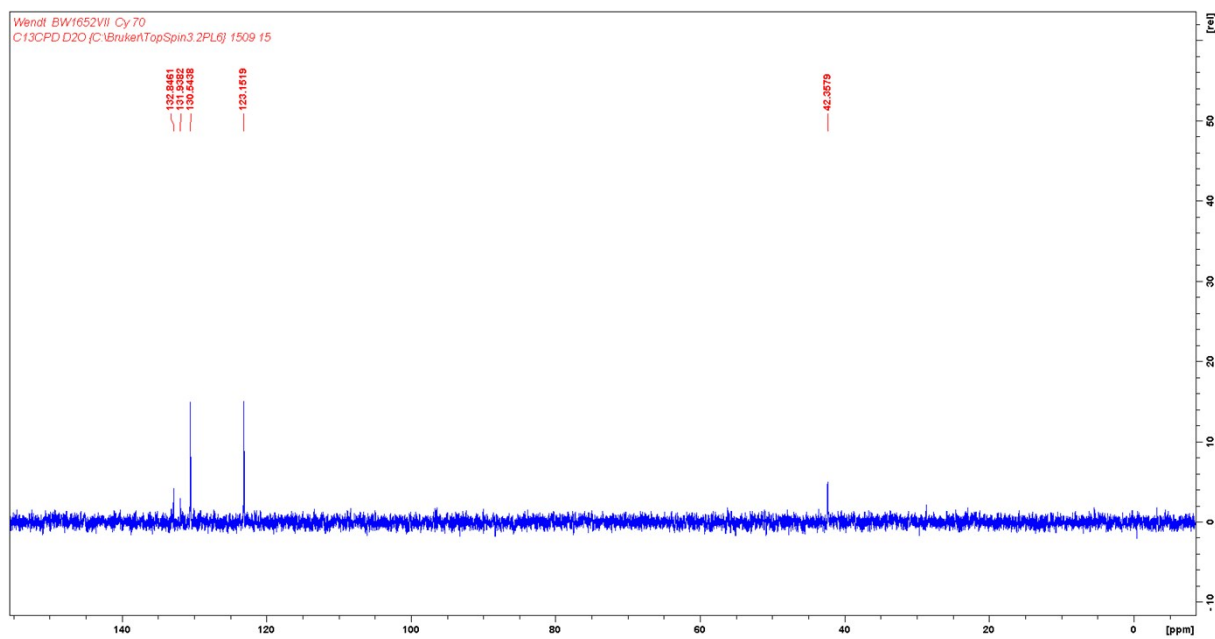
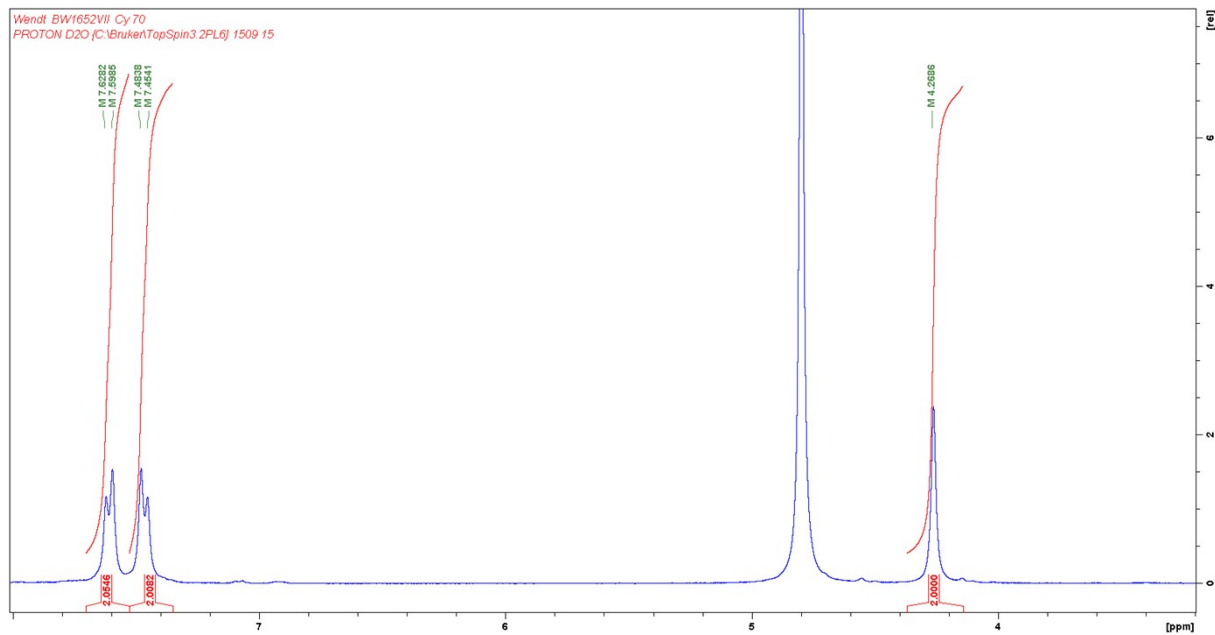


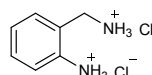
**(4-(1-hydroxyethyl)phenyl)methanaminium chloride.**  $^1\text{H}$  NMR (300.1 MHz,  $\text{D}_2\text{O}$ ),  $\delta$  = 1.49 (d, 3H), 4.20 (s, 2H), 4.89-5.31 (m, 1H), 7.20-7.74 (m, 4H).  $^{13}\text{C}$  NMR (75.5 MHz,  $\text{D}_2\text{O}$ ):  $\delta$  = 23.5, 42.7, 69.3, 126.3, 129.0, 131.7, 145.9. **GCMS-EI** (70eV):  $m/z$  (%) = 151 ( $\text{M}^+$ , 3), 150 (13), 136 (12), 119 (15), 106 (100), 91 (33), 79 (23), 77 (23), 63 (5), 51 (8), 43 (15), 30 (20).





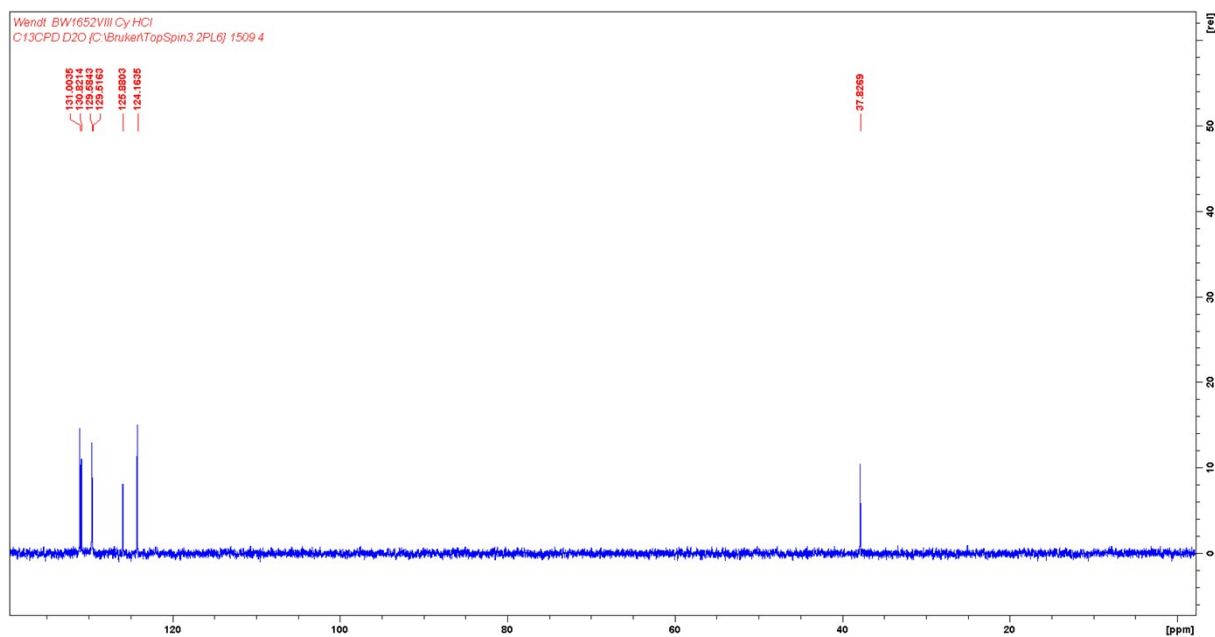
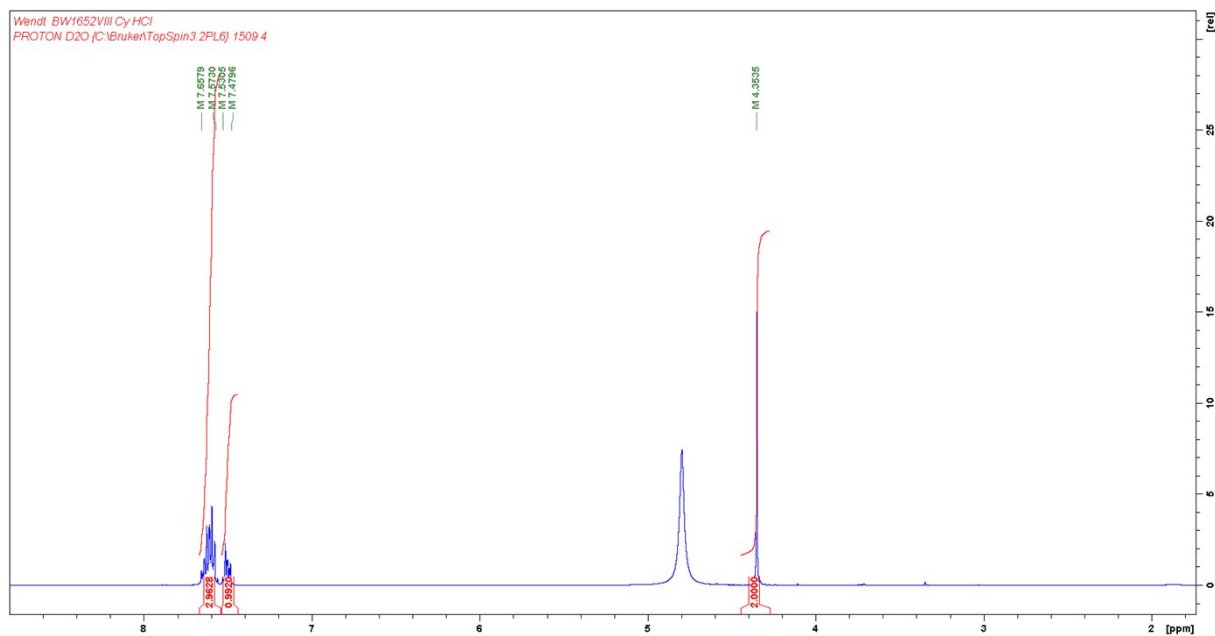
**(4-aminophenyl)methan ammonium chloride.**  $^1\text{H NMR}$  (300.1 MHz,  $\text{D}_2\text{O}$ ),  $\delta = 4.26$  (s, 2 H), 7.45-7.48 (m, 2H), 7.59-7.62 (m, 2H).  $^{13}\text{C NMR}$  (75.5 MHz,  $\text{D}_2\text{O}$ ):  $\delta = 42.3, 123.2, 130.6, 131.9, 132.8$ .





**(2-aminophenyl)methanaminium chloride.**  $^1\text{H NMR}$  (300.1 MHz,  $\text{D}_2\text{O}$ ),  $\delta =$   
 4.35 (s, 2H), 7.48-7.53 (m, 1H), 7.57-7.66 (m, 3H).  $^{13}\text{C NMR}$  (75.5 MHz,  $\text{D}_2\text{O}$ ):

$\delta = 37.8, 124.2, 125.9, 129.5, 129.6, 130.8, 131.0.$



### **Computational Details:**

Structure optimizations have been carried out at the B3PW91 [1] density functional level of theory with the all-electron TZVP basis set [2] by using the Gaussian09 program package [3]. The optimized geometries are characterized as energy minimums at the potential energy surface from frequency calculations at the same level of theory, i.e.; energy minimum structure has only real frequencies or authentic transition state have only one imaginary vibration mode, which connects the reactant and product. The Gibbs free energies which are used for discussion and comparison are scaled with the thermal correction to Gibbs free energies at 298 K. All computations have been carried out by using the Gaussian 09 program package [4].

In our study of the hydrogenation of nitrile to amine by using catalyst **1A** (without BH<sub>3</sub>) [5], we identified an outer-sphere mechanism by a simultaneous transfer of the hydride from the iron center and the proton from the nitrogen to the nitrile to give the corresponding imine based on experimental and computational analyses. The most important feature in this reaction is the reversible process between the hydrogenation and dehydrogenation of catalyst **1** and its amido intermediate **1B**. In contrast to the first step from nitrile to imine, the second step from imine to amine is barrier less, and therefore we compared only the difference in the first step. Following the same outer-sphere mechanism we computed the first step of acetonitrile and benzonitrile hydrogenation by using catalysts **2A** and **3A**, compared with that of catalyst **1A**. All these results are comparatively summarized and discussed.

[1] J. P. Perdew, *Phys. Rev. B* **1986**, 33, 8822-8824.

[2] A. Schaefer, C. Huber, R. Ahlrichs, *J. Chem. Phys.* **1994**, 100, 5829-5835.

[3] J. Frisch *et al.*, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.

[4] Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010

[5] C. Bornschein, S. Werkmeister, B. Wendt, H. Jiao, E. Alberico, H. Junge, K. Junge, M. Beller, *Nature Commun.* 2014, 5, 4111.

**Table S1.** B3PW91 computed energetic total electronic energies ( $E_{\text{tot}}$ , au), Zero-point energies (ZPE, kcal/mol, the number of imaginary frequencies (including the value of the imaginary frequencies), as well the thermal enthalpies ( $H_{\text{tot}}$ , au) and free energies ( $G_{\text{tot}}$ , au).

	B3PW91/TZVP	B3PW91/TZVP
H2	$E_{\text{tot}} = -1.1786359$ ZPE= 6.31541 NImag=0	$H_{\text{tot}} = -1,165267$ $G_{\text{tot}} = -1,180065$
Me-CN	$E_{\text{tot}} = -132.74643$ ZPE=28.43555 NImag=0	$H_{\text{tot}} = -132,696565$ $G_{\text{tot}} = -132,724084$
Me-CH=NH	$E_{\text{tot}} = -133.9497701$ ZPE= 43.00407 NImag=0	$H_{\text{tot}} = -133,876346$ $G_{\text{tot}} = -133,906200$
Ph-CN	$E_{\text{tot}} = -324,4628421$ ZPE=62.17971 NImag=0	$H_{\text{tot}} = -324.356675$ $G_{\text{tot}} = -324,393385$
Ph-CH=NH	$E_{\text{tot}} = -325,6721121$ ZPE=76.75562 NImag=0	$H_{\text{tot}} = -325.542361$ $G_{\text{tot}} = -325,580496$
Fe-Isoproyl-CO	$E_{\text{tot}} = -2747,6560051$ ZPE=337.84605 NImag=0	$H_{\text{tot}} = -2747,086713$ $G_{\text{tot}} = -2747,175333$
Fe-Isoproyl-CO-H2-TS	$E_{\text{tot}} = -2747,6216128$ ZPE=334.05204 NImag=1 (-976 cm <sup>-1</sup> )	$H_{\text{tot}} = -2747,058396$ $G_{\text{tot}} = -2747,147494$
Fe-Isopropyl-16e-CO	$E_{\text{tot}} = -2746.454005$ ZPE=324.91590 NImag=0	$H_{\text{tot}} = -2745,905471$ $G_{\text{tot}} = -2745,994751$
Fe-Isopropyl-CO+NC-Me-TS	$E_{\text{tot}} = -2880.3897829$ ZPE=365.00058 NImag= 1 (-984 cm <sup>-1</sup> )	$H_{\text{tot}} = -2879,772890$ $G_{\text{tot}} = -2879,871453$
Fe-Isopropyl-CO+NC-Ph-TS	$E_{\text{tot}} = -3072,1131822$ ZPE=399.30367 NImag=1 (-933 cm <sup>-1</sup> )	$H_{\text{tot}} = -3071.438928$ $G_{\text{tot}} = -3071,544252$
Fe-Methyl-CO.out	$E_{\text{tot}} = -2433.1880613$ ZPE=194.77033 NImag=0	$H_{\text{tot}} = -2432.857482$ $G_{\text{tot}} = -2432,923492$
Fe-Methyl-CO-H2-TS.out	$E_{\text{tot}} = -2433.1537086$ ZPE=190.97350 NImag=1 (-990 cm <sup>-1</sup> )	$H_{\text{tot}} = -2432.829322$ $G_{\text{tot}} = -2432,895260$
Fe-Methyl-CO-16E.out	$E_{\text{tot}} = -2431.9859772$ ZPE=181.59151 NImag=0	$H_{\text{tot}} = -2431.676517$ $G_{\text{tot}} = -2431,743099$
Fe-Methyl-CO+NC-Me-TS	$E_{\text{tot}} = -2565.9225396$ ZPE= 221.99595 NImag=1 (-1010 cm <sup>-1</sup> )	$H_{\text{tot}} = -2565.544424$ $G_{\text{tot}} = -2565,619683$
Fe-Methyl-CO+NC-Ph-TS	$E_{\text{tot}} = -2757.6454471$ ZPE=255.84987 NImag=1 (-969 cm <sup>-1</sup> )	$H_{\text{tot}} = -2757.210504$ $G_{\text{tot}} = -2757,293485$
Fe-Ethyl-CO.out	$E_{\text{tot}} = -2590,4267991$ ZPE=267.10848 NImag=0	$H_{\text{tot}} = -2589.975685$ $G_{\text{tot}} = -2590,053911$
Fe-Ethyl-CO-H2-TS.out	$E_{\text{tot}} = -2590.3918968$ ZPE=263.52541 NImag= 1 (-1006 cm <sup>-1</sup> )	$H_{\text{tot}} = -2589.946639$ $G_{\text{tot}} = -2590,024438$

Fe-Ethyl-CO-16E.out	E <sub>tot</sub> = -2589.2245352 ZPE=253.86598 NImag=0	H <sub>tot</sub> = -2588.794603 G <sub>tot</sub> = -2588,873254
Fe-Ethyl-CO+NC-Me-TS	E <sub>tot</sub> = -2723.1607745 ZPE=294.53505 NImag=1 (-1021 cm <sup>-1</sup> )	H <sub>tot</sub> = -2722.661708 G <sub>tot</sub> = -2722,749722
Fe-Ethyl-CO+NC-Ph-TS	E <sub>tot</sub> = -2914.8836058 ZPE=328.03760 NImag=1 (-957 cm <sup>-1</sup> )	H <sub>tot</sub> = -2914.328135 G <sub>tot</sub> = -2914,423946
Fe-Cyclohexyl-2H-CO.out	E <sub>tot</sub> = -3214,589162 ZPE=504.54213 NImag=0	H <sub>tot</sub> = -3213.747354 G <sub>tot</sub> = -3213,854305
Fe-Cyclohexyl-2H-CO-TS.out	E <sub>tot</sub> = -3214.5528196 ZPE=501.39010 NImag=0	H <sub>tot</sub> = -3213.716410 G <sub>tot</sub> = -3213,821918
Fe-Cyclohexyl-H-CO-16E	E <sub>tot</sub> = -3213.3836256 ZPE=491.90821 NImag=0	H <sub>tot</sub> = -3212.562392 G <sub>tot</sub> = -3212,668090
Fe-Cyclohexyl-CO+NC-Me-TS	E <sub>tot</sub> = -3347.3212187 ZPE= 532.23021 NImag=1 (-1038 cm <sup>-1</sup> )	H <sub>tot</sub> = -3346.431205 G <sub>tot</sub> = -3346,546424
Fe-Cyclohexyl-CO+NC-Ph-TS	E <sub>tot</sub> = -3539.0439133 ZPE=565.98653 NImag=1 (-970 cm <sup>-1</sup> )	H <sub>tot</sub> = -3538.097277 G <sub>tot</sub> = -3538,219330

**Table S2.** B3PW91 Computed Cartesian Coordinates.

Fe-Isoproyl-CO	Fe-Isopropyl-16e-CO
H 0.2811590 -1.4310411 0.0000000	H -1.0283455 -0.6733320 0.0000000
Fe -0.0290500 0.1017516 0.0000000	Fe 0.0496666 0.3534829 0.0000000
H -0.1713725 1.6596793 0.0000000	P 0.2027599 0.1498969 -2.2078963
P 0.1640087 0.1107636 -2.1951913	P 0.2027599 0.1498969 2.2078963
P 0.1640087 0.1107636 2.1951913	C 2.0249048 0.3920817 -2.4214006
C 1.9869539 0.4363649 -2.4371798	C 2.0249048 0.3920817 2.4214006
C 1.9869539 0.4363649 2.4371798	H 2.1871397 1.4735927 -2.4283925
H 2.1279534 1.5195785 -2.5028547	H 2.1871397 1.4735927 2.4283925
H 2.1279534 1.5195785 2.5028547	H 2.4274253 -0.0185295 -3.3502252
H 2.3799726 -0.0015575 -3.3574098	H 2.4274253 -0.0185295 3.3502252
H 2.3799726 -0.0015575 3.3574098	C 2.6887836 -0.2075459 -1.1919721
C 2.7108894 -0.1060590 -1.2198719	C 2.6887836 -0.2075459 1.1919721
C 2.7108894 -0.1060590 1.2198719	H 3.6979533 0.2188266 -1.0792943
H 3.7751613 0.1696111 -1.2376260	H 3.6979533 0.2188266 1.0792943
H 3.7751613 0.1696111 1.2376260	H 2.8419442 -1.2911494 -1.3382209
H 2.6467475 -1.1965830 -1.1900479	H 2.8419442 -1.2911494 1.3382209
H 2.6467475 -1.1965830 1.1900479	N 1.8949112 0.0550859 0.0000000
N 2.0602237 0.3925436 0.0000000	C -0.5721609 1.4356131 3.3386436
H 2.1132415 1.4077428 0.0000000	C -0.5721609 1.4356131 -3.3386436
C -0.6366758 1.5117994 3.1672012	H -0.4220006 2.3414374 2.7393707
C -0.6366758 1.5117994 -3.1672012	H -0.4220006 2.3414374 -2.7393707
H -0.4513222 2.3373551 2.4705604	C -0.0901419 -1.5832879 2.8836582
H -0.4513222 2.3373551 -2.4705604	C -0.0901419 -1.5832879 -2.8836582
C -0.0683573 -1.5199093 3.1128034	H 0.6322968 -2.1482338 2.2808452
C -0.0683573 -1.5199093 -3.1128034	H 0.6322968 -2.1482338 -2.2808452
H 0.7462399 -2.1070983 2.6704005	C -1.2485519 1.4951331 0.0000000
H 0.7462399 -2.1070983 -2.6704005	O -2.0921153 2.2943560 0.0000000
C -1.7360299 -0.0995304 0.0000000	C 0.2451179 -1.8027217 -4.3576461
O -2.8912966 -0.2238745 0.0000000	C 0.2451179 -1.8027217 4.3576461
C 0.1219414 -1.4956475 -4.6265843	H 1.2233332 -1.4077254 -4.6376430
C 0.1219414 -1.4956475 4.6265843	H 1.2233332 -1.4077254 4.6376430
H 1.0312796 -0.9746298 -4.9342573	H -0.5037216 -1.3465809 -5.0087517
H 1.0312796 -0.9746298 4.9342573	H -0.5037216 -1.3465809 5.0087517
H -0.7245308 -1.0216746 -5.1278647	H 0.2507262 -2.8749863 -4.5777772
H -0.7245308 -1.0216746 5.1278647	H 0.2507262 -2.8749863 4.5777772
H 0.1871184 -2.5200077 -5.0069795	C -1.4776261 -2.1302211 -2.5527923
H 0.1871184 -2.5200077 5.0069795	C -1.4776261 -2.1302211 2.5527923
C -1.3726201 -2.2135074 -2.7261287	H -2.2543936 -1.6504284 -3.1515596
C -1.3726201 -2.2135074 2.7261287	H -2.2543936 -1.6504284 3.1515596
H -2.2484267 -1.6694023 -3.0864394	H -1.7197028 -1.9813328 -1.5003253
H -2.2484267 -1.6694023 3.0864394	H -1.7197028 -1.9813328 1.5003253
H -1.4538685 -2.3126409 -1.6438863	H -1.5137868 -3.2025019 -2.7684630
H -1.4538685 -2.3126409 1.6438863	H -1.5137868 -3.2025019 2.7684630
H -1.4046721 -3.2154226 -3.1660440	C -2.0786010 1.2368337 3.4987092
H -1.4046721 -3.2154226 3.1660440	C -2.0786010 1.2368337 -3.4987092
C -2.1503593 1.3377061 3.2754821	H -2.3011411 0.3925334 4.1553864
C -2.1503593 1.3377061 -3.2754821	H -2.3011411 0.3925334 -4.1553864
H -2.4125041 0.5334888 3.9675268	H -2.5771281 1.0694838 2.5430401
H -2.4125041 0.5334888 -3.9675268	H -2.5771281 1.0694838 -2.5430401
H -2.6088323 1.1204886 2.3105516	H -2.5237287 2.1272895 3.9519599
H -2.6088323 1.1204886 -2.3105516	H -2.5237287 2.1272895 -3.9519599
H -2.6032787 2.2563804 3.6606475	C 0.1063263 1.6540186 4.6898226
H -2.6032787 2.2563804 -3.6606475	C 0.1063263 1.6540186 -4.6898226
C -0.0263994 1.8811392 4.5190419	H 1.1779384 1.8368258 4.5942660



<p>C -0.0263994 1.8811392 -4.5190419  H 1.0576446 2.0048077 4.4751931  H 1.0576446 2.0048077 -4.4751931  H -0.2481572 1.1407624 5.2882390  H -0.2481572 1.1407624 -5.2882390  H -0.4460507 2.8342886 4.8571038  H -0.4460507 2.8342886 -4.8571038</p>	<p>H 1.1779384 1.8368258 -4.5942660  H -0.0320476 0.8047444 5.3601901  H -0.0320476 0.8047444 -5.3601901  H -0.3312385 2.5300488 5.1791471  H -0.3312385 2.5300488 -5.1791471</p>
<p>Fe-Isoproyl-CO-H2-TS</p> <p>H -0.0998685 -1.2540203 0.0000000  Fe 0.0027898 0.2597130 0.0000000  P 0.2125537 0.1256941 -2.2183970  P 0.2125537 0.1256941 2.2183970  C 2.0443102 0.3304007 -2.4289269  C 2.0443102 0.3304007 2.4289269  H 2.2473392 1.4042734 -2.4687125  H 2.2473392 1.4042734 2.4687125  H 2.4208655 -0.1202666 -3.3494696  H 2.4208655 -0.1202666 3.3494696  C 2.6962852 -0.2641897 -1.1925276  C 2.6962852 -0.2641897 1.1925276  H 3.7756644 -0.0363776 -1.2058771  H 3.7756644 -0.0363776 1.2058771  H 2.6147547 -1.3685288 -1.2326412  H 2.6147547 -1.3685288 1.2326412  N 2.0807100 0.2568925 0.0000000  C -0.5125062 1.5025642 3.2778849  C -0.5125062 1.5025642 -3.2778849  H -0.3401739 2.3614287 2.6184390  H -0.3401739 2.3614287 -2.6184390  C -0.1354481 -1.5489562 2.9936105  C -0.1354481 -1.5489562 -2.9936105  H 0.6039438 -2.1621603 2.4632963  H 0.6039438 -2.1621603 -2.4632963  C -1.7278628 0.3703527 0.0000000  O -2.8858508 0.4068271 0.0000000  C 0.1259726 -1.6700572 -4.4929381  C 0.1259726 -1.6700572 4.4929381  H 1.1029603 -1.2817572 -4.7880117  H 1.1029603 -1.2817572 4.7880117  H -0.6363465 -1.1491721 -5.0761039  H -0.6363465 -1.1491721 5.0761039  H 0.0912051 -2.7236930 -4.7867741  H 0.0912051 -2.7236930 4.7867741  C -1.5150951 -2.0891157 -2.6235313  C -1.5150951 -2.0891157 2.6235313  H -2.3175738 -1.5263864 -3.1047639  H -2.3175738 -1.5263864 3.1047639  H -1.6708750 -2.0547348 -1.5454276  H -1.6708750 -2.0547348 1.5454276  H -1.6038636 -3.1301147 -2.9492545  H -1.6038636 -3.1301147 2.9492545  C -2.0221747 1.3677886 3.4719544  C -2.0221747 1.3677886 -3.4719544  H -2.2644451 0.5598687 4.1666390  H -2.2644451 0.5598687 -4.1666390  H -2.5485487 1.1805715 2.5357675</p>	<p>Fe-Isoproyl-CO-op-NCR-TS.out</p> <p>H,0,1.486754322,-0.4019783329,0.  Fe,0,0.0831875242,0.1099966731,0.  P,0,0.1333189774,-0.1234405824,2.2236662578  P,0,0.1333189774,-0.1234405824,-2.2236662578  C,0,-0.7574745265,-1.7355280221,2.441477737  C,0,-0.7574745265,-1.7355280221,-2.441477737  H,0,-1.8249312082,-1.5100345192,2.4998315657  H,0,-1.8249312082,-1.5100345192,-2.4998315657  H,0,-0.4707470883,-2.2650415251,3.3523707047  H,0,-0.4707470883,-2.2650415251,-3.3523707047  C,0,-0.4858756634,-2.558730999,1.196486488  C,0,-0.4858756634,-2.558730999,-1.196486488  H,0,-1.1495323685,-3.4357478897,1.1786036529  H,0,-1.1495323685,-3.4357478897,-1.1786036529  H,0,0.5437263713,-2.9390326038,1.202230282  H,0,0.5437263713,-2.9390326038,-1.202230282  N,0,-0.7043045304,-1.7377449233,0.  C,0,-0.8362671522,1.075227975,-3.3046816884  C,0,-0.8362671522,1.075227975,3.3046816884  H,0,-1.70005219,1.2622790781,-2.6565905808  H,0,-1.70005219,1.2622790781,2.6565905808  C,0,1.8213707236,-0.4582581928,-2.9797988913  C,0,1.8213707236,-0.4582581928,2.9797988913  H,0,2.0890475629,-1.3833431414,-2.4541456174  H,0,2.0890475629,-1.3833431414,2.4541456174  C,0,0.6659663115,1.7432677583,0.  O,0,1.0907761387,2.8228951013,0.  C,0,1.8462151436,-0.7375592101,4.4806297375  C,0,1.8462151436,-0.7375592101,-4.4806297375  H,0,1.10163805,-1.47382965,4.7896706056  H,0,1.10163805,-1.47382965,-4.7896706056  H,0,1.6827954772,0.1736198799,5.0598878037  H,0,1.6827954772,0.1736198799,-5.0598878037  H,0,2.8286746563,-1.1270629773,4.7650264734  H,0,2.8286746563,-1.1270629773,-4.7650264734  C,0,2.8590442119,0.593625637,2.5935784838  C,0,2.8590442119,0.593625637,-2.5935784838  H,0,2.6661182629,1.5536724098,3.0761536098  H,0,2.6661182629,1.5536724098,-3.0761536098  H,0,2.8756966429,0.7510015354,1.5153835247  H,0,2.8756966429,0.7510015354,-1.5153835247  H,0,3.8542129646,0.2635647178,2.9069742215  H,0,3.8542129646,0.2635647178,-2.9069742215  C,0,-0.1121788821,2.4057864932,-3.5028810565  C,0,-0.1121788821,2.4057864932,3.5028810565  H,0,0.7366375588,2.3005549308,-4.1826261154  H,0,0.7366375588,2.3005549308,4.1826261154  H,0,0.2533011267,2.8257479175,-2.5653973959</p>

<p>H -2.5485487 1.1805715 -2.5357675  H -2.4235710 2.2914613 3.8994982  H -2.4235710 2.2914613 -3.8994982  C 0.1882504 1.7836137 4.6068033  C 0.1882504 1.7836137 -4.6068033  H 1.2652741 1.9160436 4.4936691  H 1.2652741 1.9160436 -4.4936691  H 0.0213515 0.9889081 5.3350733  H 0.0213515 0.9889081 -5.3350733  H -0.2094869 2.7078555 5.0382378  H -0.2094869 2.7078555 -5.0382378  H 0.3494235 1.8859772 0.0000000  H 1.1988722 1.4222249 0.0000000</p>	<p>H,0,0.2533011267,2.8257479175,2.5653973959  H,0,-0.794465288,3.1347228923,-3.9502809673  H,0,-0.794465288,3.1347228923,3.9502809673  C,0,-1.3627707918,0.5287743904,-4.6310477717  C,0,-1.3627707918,0.5287743904,4.6310477717  H,0,-1.916926053,-0.4032456346,-4.5101848934  H,0,-1.916926053,-0.4032456346,4.5101848934  H,0,-0.5626757046,0.3562023556,-5.351817486  H,0,-0.5626757046,0.3562023556,5.351817486  H,0,-2.0478096534,1.2578760738,-5.075306504  H,0,-2.0478096534,1.2578760738,5.075306504  H,0,-1.6762144793,0.5786117049,0.  H,0,-1.9241688888,-1.4809663245,0.  N,0,-3.1521131308,-0.9389414502,0.  C,0,-2.845241371,0.2479591562,0.  C,0,-3.6748489732,1.4975623837,0.  H,0,-4.7347830657,1.2423963061,0.  H,0,-3.4473452972,2.1095300525,-0.8780158015  H,0,-3.4473452972,2.1095300525,0.8780158015</p>
<p>H,0,2.2395085235,0.2595548991,0.  Fe,0,0.7627202718,0.0562392385,0.  P,0,0.9215243711,-0.1323981106,2.2252194534  P,0,0.9215243711,-0.1323981106,-2.2252194534  C,0,0.8478668989,-1.9720673107,2.4407562283  C,0,0.8478668989,-1.9720673107,-2.4407562283  H,0,-0.2080615084,-2.2487347626,2.493998745  H,0,-0.2080615084,-2.2487347626,-2.493998745  H,0,1.3361452906,-2.3182532217,3.3540348889  H,0,1.3361452906,-2.3182532217,-3.3540348889  C,0,1.4651146743,-2.5876578059,1.1986115364  C,0,1.4651146743,-2.5876578059,-1.1986115364  H,0,1.2633951048,-3.6686018694,1.179326077  H,0,1.2633951048,-3.6686018694,-1.179326077  H,0,2.5560476746,-2.4682182986,1.2072360858  H,0,2.5560476746,-2.4682182986,-1.2072360858  N,0,0.9048316178,-1.9514221156,0.  C,0,-0.4744335137,0.5035985434,-3.3140709754  C,0,-0.4744335137,0.5035985434,3.3140709754  H,0,-1.3386674632,0.2780975427,-2.6788578309  H,0,-1.3386674632,0.2780975427,2.6788578309  C,0,2.5875730469,0.3193140243,-2.9654237859  C,0,2.5875730469,0.3193140243,2.9654237859  H,0,3.2352636642,-0.3810761377,-2.4236568551  H,0,3.2352636642,-0.3810761377,2.4236568551  C,0,0.5450399652,1.7741926085,0.  O,0,0.4400487647,2.9298770203,0.  C,0,2.7545329534,0.0621340798,4.4616186729  C,0,2.7545329534,0.0621340798,-4.4616186729  H,0,2.4236069974,-0.9337475881,4.7626110467  H,0,2.4236069974,-0.9337475881,-4.7626110467  H,0,2.2072729356,0.7952864281,5.0577904847  H,0,2.2072729356,0.7952864281,-5.0577904847  H,0,3.8110508054,0.1518468475,4.7327908315  H,0,3.8110508054,0.1518468475,-4.7327908315  C,0,3.0415222837,1.7293771792,2.5928229391</p>	

<p>C,0,3.0415222837,1.7293771792,-2.5928229391  H,0,2.4451606405,2.495538168,3.0918543118  H,0,2.4451606405,2.495538168,-3.0918543118  H,0,2.9768988026,1.8934144487,1.5174174719  H,0,2.9768988026,1.8934144487,-1.5174174719  H,0,4.08223985,1.8743810735,2.8980752817  H,0,4.08223985,1.8743810735,-2.8980752817  C,0,-0.4253123453,2.0186579125,-3.5049963349  C,0,-0.4253123453,2.0186579125,3.5049963349  H,0,0.3808632709,2.3090227511,-4.1826815998  H,0,0.3808632709,2.3090227511,4.1826815998  H,0,-0.2884115996,2.5542463885,-2.5650519532  H,0,-0.2884115996,2.5542463885,2.5650519532  H,0,-1.3625465081,2.3641175295,-3.9508191512  H,0,-1.3625465081,2.3641175295,3.9508191512  C,0,-0.6844364788,-0.2137458454,-4.647338312  C,0,-0.6844364788,-0.2137458454,4.647338312  H,0,-0.7547894122,-1.2967251546,-4.5350977878  H,0,-0.7547894122,-1.2967251546,4.5350977878  H,0,0.1114750122,0.0026772534,-5.3609259041  H,0,0.1114750122,0.0026772534,5.3609259041  H,0,-1.623731389,0.1269123726,-5.0938767899  H,0,-1.623731389,0.1269123726,5.0938767899  H,0,-1.0322005908,-0.3386282983,0.  H,0,-0.2901026745,-2.2781334916,0.  N,0,-1.6355593656,-2.3672389113,0.  C,0,-1.9065026924,-1.1664943716,0.  C,0,-3.2101980904,-0.4660915647,0.  C,0,-3.2767524198,0.9251305785,0.  C,0,-4.5066260129,1.572050505,0.  C,0,-5.6805192744,0.8299945364,0.  C,0,-4.3949834912,-1.2074740479,0.  C,0,-5.6204341553,-0.5617371331,0.  H,0,-2.3553943606,1.4992781281,0.  H,0,-4.5476962395,2.6558467347,0.  H,0,-6.641644075,1.3325837215,0.  H,0,-4.3240219676,-2.2892055001,0.  H,0,-6.5364870084,-1.1427347389,0.</p>	
<p>Fe-Methyl-CO.out</p> <p>H,0,-0.4004094489,0,-1.485666222  Fe,0,-0.6418480024,0,0.0581979241  H,0,-0.7281012507,0,1.619426737  C,0,-2.3574763548,0,-0.1058773412  O,0,-3.511807963,0,-0.2160759784  P,0,-0.4597767142,2.1640511829,0.0537915634  P,0,-0.4597767142,-2.1640511829,0.0537915634  C,0,1.3713472601,2.4458007978,0.2802457161  C,0,1.3713472601,-2.4458007978,0.2802457161  H,0,1.5637484929,2.5482751308,1.3528598913  H,0,1.5637484929,-2.5482751308,1.3528598913  H,0,1.7203522146,3.3594259158,-0.2071749597  H,0,1.7203522146,-3.3594259158,-0.2071749597  C,0,2.0814388824,1.2216138313,-0.2705979638  C,0,2.0814388824,-1.2216138313,-0.2705979638  H,0,3.1551005282,1.2457190579,-0.0366427294  H,0,3.1551005282,-1.2457190579,-0.0366427294</p>	<p>Fe-Methyl-CO-H2-TS.out</p> <p>H,0,-0.047397765,-1.4910677089,0.  Fe,0,0.3385505185,-0.0238466054,0.  C,0,2.0129295641,-0.4893873019,0.  O,0,3.1164160397,-0.834915903,0.  P,0,0.0896246735,-0.1123295763,2.1806056322  P,0,0.0896246735,-0.1123295763,-2.1806056322  C,0,-1.5631247378,0.6834243351,2.4398425311  C,0,-1.5631247378,0.6834243351,-2.4398425311  H,0,-1.3908664039,1.759998778,2.5282723768  H,0,-1.3908664039,1.759998778,-2.5282723768  H,0,-2.0569257806,0.3397205726,3.3521314124  H,0,-2.0569257806,0.3397205726,-3.3521314124  C,0,-2.3840616034,0.3854542409,1.1939647195  C,0,-2.3840616034,0.3854542409,-1.1939647195  H,0,-3.3106101111,0.9830724504,1.2163781294  H,0,-3.3106101111,0.9830724504,-1.2163781294  H,0,-2.7021070072,-0.6752651882,1.2182391588</p>

<p>H,0,1.9730657532,1.1801040031,-1.3571872136  H,0,1.9730657532,-1.1801040031,-1.3571872136  N,0,1.4548505785,0,0.2623201533  H,0,1.557400081,0,1.2737120405  C,0,-1.2124830864,-3.2193150592,1.367114431  C,0,-1.2124830864,3.2193150592,1.367114431  H,0,-2.2987762435,-3.18516574,1.2656425552  H,0,-2.2987762435,3.18516574,1.2656425552  H,0,-0.9546979578,-2.8011520545,2.3404183082  H,0,-0.9546979578,2.8011520545,2.3404183082  H,0,-0.8812641224,-4.2587971474,1.3058682437  H,0,-0.8812641224,4.2587971474,1.3058682437  C,0,-0.8652826338,-3.1363364881,-1.4630447533  C,0,-0.8652826338,3.1363364881,-1.4630447533  H,0,-1.9297489369,-3.0219374281,-1.6757611172  H,0,-1.9297489369,3.0219374281,-1.6757611172  H,0,-0.6317137466,-4.1982270221,-1.3521319702  H,0,-0.6317137466,4.1982270221,-1.3521319702  H,0,-0.3138671466,-2.7175056369,-2.3052525282  H,0,-0.3138671466,2.7175056369,-2.3052525282</p>	<p>H,0,-2.7021070072,-0.6752651882,-1.2182391588  N,0,-1.6243005086,0.6666044515,0.  C,0,1.213677249,0.7962578538,-3.3262589078  C,0,1.213677249,0.7962578538,3.3262589078  H,0,2.2056730327,0.3422546091,-3.2955109781  H,0,2.2056730327,0.3422546091,3.2955109781  H,0,1.3039532244,1.8303427045,-2.9912771897  H,0,1.3039532244,1.8303427045,2.9912771897  H,0,0.8446402572,0.7777259056,-4.354299128  H,0,0.8446402572,0.7777259056,4.354299128  C,0,-0.0390226261,-1.7576750501,-2.9956196381  C,0,-0.0390226261,-1.7576750501,2.9956196381  H,0,0.9029411461,-2.2933287579,-2.867114842  H,0,0.9029411461,-2.2933287579,2.867114842  H,0,-0.2625266978,-1.6641115389,-4.0609277459  H,0,-0.2625266978,-1.6641115389,4.0609277459  H,0,-0.8219465798,-2.3335643198,-2.502237438  H,0,-0.8219465798,-2.3335643198,2.502237438  H,0,-0.4059325702,1.4683553523,0.  H,0,0.551646664,1.6229510696,0.</p>
<p>Fe-Methyl-CO-16E.out</p> <p>H,0,1.1649038881,-0.9945147256,0.  Fe,0,0.2770811275,0.203648335,0.  C,0,1.7626377204,1.103489424,0.  O,0,2.7491682463,1.7130875884,0.  P,0,0.1079511997,-0.0063673786,2.1734352847  P,0,0.1079511997,-0.0063673786,-2.1734352847  C,0,-1.6943980734,0.3028948465,2.4388305265  C,0,-1.6943980734,0.3028948465,-2.4388305265  H,0,-1.8157696796,1.3874208202,2.506437064  H,0,-1.8157696796,1.3874208202,-2.506437064  H,0,-2.0809212165,-0.1474730119,3.3570804287  H,0,-2.0809212165,-0.1474730119,-3.3570804287  C,0,-2.3923887841,-0.2183474554,1.1909614049  C,0,-2.3923887841,-0.2183474554,-1.1909614049  H,0,-3.3799612615,0.258509388,1.0946819041  H,0,-3.3799612615,0.258509388,-1.0946819041  H,0,-2.5936108759,-1.2983946985,1.3016916806  H,0,-2.5936108759,-1.2983946985,-1.3016916806  N,0,-1.589916415,0.0413858569,0.  C,0,0.9614156714,1.0793149702,-3.3935433985  C,0,0.9614156714,1.0793149702,3.3935433985  H,0,2.0375431178,0.9055518546,-3.3421383284  H,0,2.0375431178,0.9055518546,3.3421383284  H,0,0.7754526473,2.1232813082,-3.137899392  H,0,0.7754526473,2.1232813082,3.137899392  H,0,0.6167435581,0.8886915476,-4.4124515956  H,0,0.6167435581,0.8886915476,4.4124515956  C,0,0.4014402635,-1.6860497275,-2.8752458582  C,0,0.4014402635,-1.6860497275,2.8752458582  H,0,1.4556183022,-1.940130235,-2.7563224633  H,0,1.4556183022,-1.940130235,2.7563224633  H,0,0.1298500103,-1.7396497242,-3.9321124647  H,0,0.1298500103,-1.7396497242,3.9321124647  H,0,-0.1834859345,-2.4109356288,-2.3080428778</p>	<p>Fe-Methyl-CO-NCR-TS.out</p> <p>H,0,0.6507857285,-1.727885876,0.0005780293  Fe,0,0.4567247499,-0.2462843365,-0.0002082456  P,0,0.2822586893,-0.4233406526,2.1844244305  P,0,0.280139096,-0.4259163412,-2.1844369095  C,0,-1.5486159707,-0.4007636515,2.4560591549  C,0,-1.5509893994,-0.4038619424,-2.454380599  H,0,-1.8430745433,0.6449578773,2.575375443  H,0,-1.8456625137,0.6416736927,-2.5748064525  H,0,-1.8496685751,-0.9464007691,3.3536872388  H,0,-1.8528302419,-0.9507020163,-3.3510105874  C,0,-2.1804139534,-0.9743640311,1.198614754  C,0,-2.1815392109,-0.9758830064,-1.1955885971  H,0,-3.2594540308,-0.7636778029,1.1929918849  H,0,-3.2605816266,-0.7652279908,-1.1891808193  H,0,-2.0691547526,-2.0660929607,1.1809420757  H,0,-2.0702248018,-2.067585006,-1.1766647392  N,0,-1.5496499012,-0.3976267324,0.0008507832  C,0,0.9211566075,0.852965603,-3.3492599083  C,0,0.9245555782,0.856769582,3.3471891582  H,0,2.0108603885,0.8793892054,-3.2954653766  H,0,2.0142111515,0.882992308,3.2923279881  H,0,0.5391892009,1.8298292983,-3.0511259111  H,0,0.542425821,1.8333497159,3.0483356385  H,0,0.6195907077,0.6479699064,-4.3790004363  H,0,0.6239445279,0.6529613053,4.377444503  C,0,0.8659612539,-1.9830753882,-2.9760977805  C,0,0.8686410333,-1.9796546384,2.9773217052  H,0,1.947211532,-2.0606702783,-2.8508158255  H,0,1.9497396652,-2.0576123255,2.8509616691  H,0,0.621935779,-2.0108390385,-4.0404541602  H,0,0.6257640921,-2.006087034,4.041974826  H,0,0.4082212477,-2.833018456,-2.4698059337  H,0,0.410189355,-2.8301234387,2.4725580127  C,0,2.18052022,-0.0309349892,-0.0011417479  O,0,3.3341540312,0.0700301896,-0.0017181309</p>

<p>H,0,-0.1834859345,-2.4109356288,2.3080428778</p>	<p>H,0,0.0817960295,1.5195336827,-0.0012609835  H,0,-1.8773043496,0.8043038949,0.000281515  C,0,-0.7513651835,2.4101230091,-0.0009929952  N,0,-1.947031312,2.1439823103,-0.0001810423  C,0,-0.0106273018,3.7136837957,-0.001889851  H,0,-0.716273632,4.5447787005,-0.0013101643  H,0,0.6389705225,3.785065719,0.8754163709  H,0,0.637184592,3.7848356065,-0.8805379839</p>
<p>Fe-Methyl-CO-NC-Ph-TS.out</p> <p>H,0,0.,0.7950022437,-2.5140274295  Fe,0,0.,0.4385649968,-1.0656055238  P,0,2.190205925,0.2780605522,-1.2437940283  P,0,-2.190205925,0.2780605522,-1.2437940283  C,0,2.453178582,-1.5430380303,-1.4451238148  C,0,-2.453178582,-1.5430380303,-1.4451238148  H,0,2.5653746997,-1.9654925081,-0.4434328303  H,0,-2.5653746997,-1.9654925081,-0.4434328303  H,0,3.3532035049,-1.7784625053,-2.0182338656  H,0,-3.3532035049,-1.7784625053,-2.0182338656  C,0,1.1977371186,-2.0929515001,-2.1006330381  C,0,-1.1977371186,-2.0929515001,-2.1006330381  H,0,1.1882715886,-3.1899441836,-2.0296046634  H,0,-1.1882715886,-3.1899441836,-2.0296046634  H,0,1.1840741227,-1.8417860936,-3.1687401327  H,0,-1.1840741227,-1.8417860936,-3.1687401327  N,0,0.,-1.5368972896,-1.4517783274  C,0,-3.3359394782,0.755392804,0.1187847774  C,0,3.3359394782,0.755392804,0.1187847774  H,0,-3.3028612475,1.837484703,0.2571307148  H,0,3.3028612475,1.837484703,0.2571307148  H,0,-3.0086770298,0.2823396023,1.0452983039  H,0,3.0086770298,0.2823396023,1.0452983039  H,0,-4.3634988727,0.4544669578,-0.0978367342  H,0,4.3634988727,0.4544669578,-0.0978367342  C,0,-2.9955097846,1.0469879545,-2.7111525342  C,0,2.9955097846,1.0469879545,-2.7111525342  H,0,-2.8545745488,2.1281779642,-2.6679209917  H,0,2.8545745488,2.1281779642,-2.6679209917  H,0,-4.0638247592,0.8223162519,-2.7485763318  H,0,4.0638247592,0.8223162519,-2.7485763318  H,0,-2.5096654222,0.6815479735,-3.6160601225  H,0,2.5096654222,0.6815479735,-3.6160601225  C,0,0.,2.1345626024,-0.6938322511  O,0,0.,3.276755777,-0.5014933005  H,0,0.,-0.1431292382,0.665763094  H,0,0.,-2.0032903703,-0.3016898333  C,0,0.,-1.0766781407,1.4330869974  N,0,0.,-2.2364832996,1.0226987427  C,0,0.,-0.5330280781,2.8090555168  C,0,0.,0.8409309763,3.0368731  C,0,0.,1.3402888151,4.333567872  C,0,0.,0.466645422,5.4131690486  C,0,0.,-1.4075825574,3.899287922  C,0,0.,-0.9085770281,5.191491684  H,0,0.,1.5176194019,2.1878539353  H,0,0.,2.41191265,4.5004656406</p>	

H,0,0.,0.8536955025,6.4263299536 H,0,0.,-2.4738137972,3.7035866204 H,0,0.,-1.5923710892,6.0335982161	
Fe-Ethyl-CO  H -2.5534372293,1.3751341935,2.2216034884 H -2.5674965845,2.152439342,3.8078759049 H -2.4850323055,0.3965821463,3.6877958511 H 0.4023259828,-1.4566331994,0.003120018 Fe 0.0067700842,0.055253309,0.00191712 H -0.2411162276,1.6023410475,0.0007070057 P 0.1892925537,0.0998578019,-2.1703919533 P 0.1885269941,0.1031669487,2.1742205833 C 2.0018802809,0.4609834804,-2.4439729492 C 2.0009522389,0.4649711542,2.4478743821 H 2.1105312131,1.54461818,-2.5537646303 H 2.1094064186,1.5488075428,2.5558654723 H 2.3968331507,0.0014758121,-3.3526819486 H 2.3956796783,0.007066349,3.357491385 C 2.7497753599,-0.0255004949,-1.2166621819 C 2.7493450485,-0.02346808,1.2216395103 H 3.800033167,0.2987598041,-1.2373363293 H 3.7995772375,0.3008826903,1.2421779024 H 2.7342586807,-1.1172140442,-1.1729246911 H 2.7339117952,-1.1152537932,1.1796798983 N 2.0774275187,0.4528983206,0.0019730008 H 2.0906048194,1.469494464,0.0011290141 C -0.6207646597,1.4218633404,3.2020937808 C -0.6194247136,1.4171576609,-3.2005113713 H -0.3162937268,2.3636066981,2.7376853497 H -0.3151093016,2.3595181571,-2.7372490143 C -0.1220438516,-1.4568879925,3.1389421618 C -0.1211501232,-1.4616302851,-3.1328691433 H 0.5163191952,-2.2061132011,2.6627155924 H 0.5167690282,-2.2102652715,-2.6551319131 C -1.6654034612,-0.3575070737,0.0019163371 O -2.7839507431,-0.6670563221,0.0019343361 C 0.0868619203,-1.4333187428,-4.6412269781 C 0.08506701,-1.4262055222,4.6473692813 H 1.1007588782,-1.1269391904,-4.9121114728 H 1.0986873023,-1.1190270518,4.9183990251 H -0.6073813747,-0.7511944268,-5.1363996893 H -0.6097141781,-0.743584636,5.1411133145 H -0.0741101833,-2.4268466149,-5.0688902166 H -0.0757714573,-2.419140076,5.0764566283 H -1.1446014834,-1.759587599,-2.8872762989 C -2.1413133214,1.3277815423,3.2306702002 C -2.1399591829,1.3231341254,-3.2296889384 H -2.4835134311,0.3913562766,-3.6857622138 H -2.5525553131,1.3718289141,-2.2208793631 H -2.5658188652,2.147062518,-3.8081757321 H -0.2068595889,1.4048991444,4.2155482527 H -0.2050416707,1.3987752893,-4.2137410425 H -1.1452989785,-1.7554474356,2.8932365745	Fe-Ethyl-CO-H2-TS  H 0.2556391669,-1.335397881,0. Fe -0.1284442428,0.1333050918,0. P 0.1150191711,0.0659708231,-2.1936140388 P 0.1150191711,0.0659708231,2.1936140388 C 1.7926310951,0.8172196572,-2.4391031222 C 1.7926310951,0.8172196572,2.4391031222 H 1.6459369347,1.8977333965,-2.5289965341 H 1.6459369347,1.8977333965,2.5289965341 H 2.2884067447,0.4685827599,-3.347888161 H 2.2884067447,0.4685827599,3.347888161 C 2.5981964901,0.5005032826,-1.1905555975 C 2.5981964901,0.5005032826,1.1905555975 H 3.5413475799,1.0719910613,-1.2094562599 H 3.5413475799,1.0719910613,1.2094562599 H 2.886208706,-0.5690263848,-1.210474701 H 2.886208706,-0.5690263848,1.210474701 N 1.8431434607,0.8042825755,0. C -0.942937215,1.0713385358,3.3422671194 C -0.942937215,1.0713385358,-3.3422671194 H -0.8995200575,2.0924765041,2.9527779443 H -0.8995200575,2.0924765041,-2.9527779443 C 0.1909825265,-1.6087814923,2.9867046802 C 0.1909825265,-1.6087814923,-2.9867046802 H 0.9576658914,-2.1469972932,2.4232416955 H 0.9576658914,-2.1469972932,-2.4232416955 C -1.7881647238,-0.3756989725,0. O -2.8743802605,-0.7760167648,0. C 0.4610745736,-1.6695719344,-4.4842885792 C 0.4610745736,-1.6695719344,4.4842885792 H 1.3949553444,-1.169785997,-4.7528354199 H 1.3949553444,-1.169785997,4.7528354199 H -0.3409031061,-1.2086584733,-5.0646687163 H -0.3409031061,-1.2086584733,5.0646687163 H 0.5440480464,-2.7087771119,-4.8135618314 H 0.5440480464,-2.7087771119,4.8135618314 H -0.7524272979,-2.1020812115,-2.7364718236 H -0.7524272979,-2.1020812115,2.7364718236 C -2.3919422033,0.6106678942,3.4467346283 C -2.3919422033,0.6106678942,-3.4467346283 H -2.4701493177,-0.4084007645,3.8331987483 H -2.4701493177,-0.4084007645,-3.8331987483 H -2.8903281121,0.634698487,2.4768034884 H -2.8903281121,0.634698487,-2.4768034884 H -2.9511001153,1.2600306622,4.125232575 H -2.9511001153,1.2600306622,-4.125232575 H -0.4681554122,1.0862953903,4.3283967674 H -0.4681554122,1.0862953903,-4.3283967674 H -0.325349274,1.7816686664,0. H 0.6352355227,1.6168973109,0.
Fe-Ethyl-CO-16E  H 0.9223585166,-0.9348944565,0.	Fe-Ethyl-CO-op-NCR-TS.out  H,0,0.0983683517,-1.6890886455,-0.0013363422

<p>Fe 0.1269759178,0.3329076333,0.  C 1.6652067579,1.1276206273,0.  O 2.6777628899,1.6963268978,0.  P -0.081620638,0.1044941831,2.1743031668  P -0.081620638,0.1044941831,-2.1743031668  C -1.7880066874,0.760839674,2.4411529962  C -1.7880066874,0.760839674,-2.4411529962  H -1.6841293774,1.8468731031,2.5172623589  H -1.6841293774,1.8468731031,-2.5172623589  H -2.2653153578,0.3995916548,3.3552851833  H -2.2653153578,0.3995916548,-3.3552851833  C -2.578642498,0.4033979359,1.190560133  C -2.578642498,0.4033979359,-1.190560133  H -3.4388310916,1.0835690698,1.0920556697  H -3.4388310916,1.0835690698,-1.0920556697  H -3.0118593122,-0.606310013,1.3000187665  H -3.0118593122,-0.606310013,-1.3000187665  N -1.7386139402,0.4811774399,0.  C 0.9450801295,0.985893724,-3.4435885938  C 0.9450801295,0.985893724,3.4435885938  C 2.3797539427,0.4788410707,-3.5423745922  C 2.3797539427,0.4788410707,3.5423745922  H 0.9364737143,2.0391603664,-3.1493228954  H 0.9364737143,2.0391603664,3.1493228954  H 0.4412156034,0.9215025246,-4.4130312817  H 0.4412156034,0.9215025246,4.4130312817  C -0.1271362823,-1.6553426539,-2.7679898021  C -0.1271362823,-1.6553426539,2.7679898021  H 0.8584728406,-2.0686003004,-2.537971675  H 0.8584728406,-2.0686003004,2.537971675  C -0.5011880145,-1.9025188146,-4.2239177804  C -0.5011880145,-1.9025188146,4.2239177804  H -0.819587857,-2.1634681636,-2.0912576053  H -0.819587857,-2.1634681636,2.0912576053  H 2.9455981032,1.0718978469,-4.2652268561  H 2.9455981032,1.0718978469,4.2652268561  H 2.8938914798,0.5467862296,-2.582558155  H 2.8938914798,0.5467862296,2.582558155  H 2.4195802574,-0.5622075185,-3.8711215855  H 2.4195802574,-0.5622075185,3.8711215855  H -0.5153868423,-2.9747966558,4.4376774031  H -0.5153868423,-2.9747966558,-4.4376774031  H 0.2114878238,-1.4440378729,4.9129991513  H 0.2114878238,-1.4440378729,-4.9129991513  H -1.4928295287,-1.511647406,4.463405475  H -1.4928295287,-1.511647406,-4.463405475</p>	<p>Fe,0,0.1693295072,-0.1965789309,-0.0001940361  P,0,-0.0372430113,-0.3270297886,2.1979354576  P,0,-0.0386957198,-0.3236387501,-2.1983836121  C,0,-1.8456590043,-0.0222346285,2.454821705  C,0,-1.8473337098,-0.0187612691,-2.4536287214  H,0,-1.9692142321,1.0569909301,2.5770062986  H,0,-1.9711334937,1.0606090784,-2.5742695725  H,0,-2.2420678566,-0.5092630912,3.3484122415  H,0,-2.2442555001,-0.504636115,-3.3476202787  C,0,-2.5565736525,-0.4827519218,1.1946426025  C,0,-2.5573505691,-0.4811129547,-1.1936143784  H,0,-3.5869255212,-0.098859135,1.1859040882  H,0,-3.5877254448,-0.0973115878,-1.1836325216  H,0,-2.6257302171,-1.5781618072,1.1744656526  H,0,-2.6264099907,-1.5765546089,-1.1749390561  N,0,-1.8370810521,-0.0148539919,0.0006001342  C,0,0.7396853773,0.8930053268,-3.3672579257  C,0,0.7421244997,0.8876604449,3.3681797483  C,0,2.2582131714,0.8035166372,-3.458851618  C,0,2.2607105165,0.7978743959,3.4585413571  H,0,0.4368502958,1.8786673905,-3.0035033932  H,0,0.439142335,1.8739303844,3.0061982828  H,0,0.2822530028,0.7680729856,-4.3536812483  H,0,0.285386702,0.7612280435,4.3547336619  C,0,0.3176968825,-1.9758104464,-2.9653340596  C,0,0.3193410804,-1.980461535,2.9620775305  H,0,1.3583490239,-2.2022068649,-2.716617708  H,0,1.3598110228,-2.2066355949,2.7124015277  C,0,0.0682305122,-2.1305400265,-4.4598724139  C,0,0.0707308512,-2.1375015653,4.4565193845  H,0,-0.2794954744,-2.6872980317,-2.389108195  H,0,-0.27830042,-2.6909589612,2.3850958893  C,0,1.8991035668,-0.3250479078,-0.0008739074  O,0,3.0483086502,-0.4775316282,-0.0013836951  H,0,0.1003787821,1.6024874688,0.001263892  H,0,-1.9576654351,1.2270941059,0.0015075491  C,0,-0.5730810888,2.6190284807,0.0021347366  N,0,-1.7966609616,2.5584553695,0.0024084491  C,0,0.3751480446,3.7807778356,0.0027139689  H,0,-0.1819037311,4.7179809468,0.003229823  H,0,1.0263813538,3.7422581664,0.8809146452  H,0,1.0263563621,3.7431784525,-0.8755426855  H,0,2.6460209054,1.5669181307,-4.1380873721  H,0,2.6490974307,1.5603229368,4.1385161773  H,0,2.7285768224,0.9525146308,-2.4858229262  H,0,2.730379209,0.9481290339,2.4853701022  H,0,2.5868178017,-0.1669531598,-3.8380417629  H,0,2.5894876419,-0.1731352404,3.836195195  H,0,0.2670862677,-3.1588794479,-4.7733158355  H,0,0.2699665529,-3.1662742619,4.7682953588  H,0,-0.9664865658,-1.9051049708,-4.7292011895  H,0,-0.9638819121,-1.9126796315,4.7267523078  H,0,0.7148131551,-1.480534073,-5.0529476729  H,0,0.7175096854,-1.4882659023,5.0502243606</p>
<p>"Fe-Ethyl-CO-op-NC-Ph-TS.out"  H,0,0.,0.5644782289,-2.3399184925</p>	

Fe,0,0,0.231972804,-0.8863765551  
P,0,2.2019423345,0.0649541741,-1.0676377534  
P,0,-2.2019423345,0.0649541741,-1.0676377534  
C,0,2.4520706254,-1.7618483075,-1.2413864539  
C,0,-2.4520706254,-1.7618483075,-1.2413864539  
H,0,2.5632519592,-2.1646309108,-0.2314155791  
H,0,-2.5632519592,-2.1646309108,-0.2314155791  
H,0,3.3501723229,-2.0191568562,-1.807380065  
H,0,-3.3501723229,-2.0191568562,-1.807380065  
C,0,1.1956729051,-2.3193949716,-1.8852631427  
C,0,-1.1956729051,-2.3193949716,-1.8852631427  
H,0,1.18410945,-3.4152422515,-1.7958921551  
H,0,-1.18410945,-3.4152422515,-1.7958921551  
H,0,1.1815966359,-2.0872931031,-2.9578052622  
H,0,-1.1815966359,-2.0872931031,-2.9578052622  
N,0,0,-1.751476498,-1.2453932273  
C,0,-3.3783496707,0.5108214177,0.2973312816  
C,0,3.3783496707,0.5108214177,0.2973312816  
C,0,-3.5031790329,2.0053943048,0.5692323118  
C,0,3.5031790329,2.0053943048,0.5692323118  
H,0,-3.0034714425,-0.0053463786,1.1853442374  
H,0,3.0034714425,-0.0053463786,1.1853442374  
H,0,-4.3558707513,0.0755846426,0.0671091854  
H,0,4.3558707513,0.0755846426,0.0671091854  
C,0,-2.9530729479,0.8219845751,-2.587194721  
C,0,2.9530729479,0.8219845751,-2.587194721  
H,0,-2.7001009228,1.8851499091,-2.5498435228  
H,0,2.7001009228,1.8851499091,-2.5498435228  
C,0,-4.4466167241,0.6231551879,-2.8085880414  
C,0,4.4466167241,0.6231551879,-2.8085880414  
H,0,-2.3726445091,0.4145912728,-3.4191633919  
H,0,2.3726445091,0.4145912728,-3.4191633919  
C,0,0,1.9368508794,-0.5688022421  
O,0,0,3.0875862425,-0.4281969668  
H,0,0,-0.331032688,0.8576261619  
H,0,0,-2.2012539802,-0.0898425317  
C,0,0,-1.2549909376,1.6343603876  
N,0,0,-2.4198956591,1.2378264784  
C,0,0,-0.6982263001,3.0052867893  
H,0,-4.1843697951,2.1836921203,1.404844378  
H,0,4.1843697951,2.1836921203,1.404844378  
H,0,-2.540651563,2.4496216378,0.8261548994  
H,0,2.540651563,2.4496216378,0.8261548994  
H,0,-3.8966098562,2.5467882614,-0.2943440167  
H,0,3.8966098562,2.5467882614,-0.2943440167  
H,0,-4.7497726986,1.0566005929,-3.7653392013  
H,0,4.7497726986,1.0566005929,-3.7653392013  
H,0,-4.7209221132,-0.4341850937,-2.8305864942  
H,0,4.7209221132,-0.4341850937,-2.8305864942  
H,0,-5.0433283798,1.1044471634,-2.0312641493  
H,0,5.0433283798,1.1044471634,-2.0312641493  
C,0,0,0.6776700933,3.2193010674  
C,0,0,1.1906648906,4.510688857  
C,0,0,0.328088935,5.5992233034  
C,0,0,-1.5614771926,4.1043799813  
C,0,0,-1.049293753,5.3914849731  
H,0,0,1.3441691241,2.3621858739



<p>H,0,0.,2.2639329859,4.6668966523  H,0,0.,0.7253846256,6.6084125747  H,0,0.,-2.6296142303,3.9191813908  H,0,0.,-1.7245352351,6.2404980157</p>	
<p>Fe-Cyclohexyl-2H-CO</p> <p>H -1.3133501658,-2.2742812524,0.0000000004  N -0.2976359064,-2.2366024255,0.0000000003  Fe 0.0229476225,-0.1492394588,0.0000000003  H -1.533774045,0.0145116205,0.0000000004  P -0.020531711,-0.3399662348,2.1905759295  P -0.0205317113,-0.3399662348,-2.1905759288  C 0.2820901874,1.5525980628,0.0000000003  O 0.4552547662,2.7005256434,0.0000000003  H 1.5496037925,-0.4667462985,0.0000000002  C -0.3112728254,-2.1720887399,-2.4449159312  C -0.3112728251,-2.1720887399,2.4449159318  H -1.3906766936,-2.3175709916,-2.55247907  H -1.3906766933,-2.3175709917,2.5524790708  H 0.159150203,-2.557518616,-3.3517750232  H 0.1591502034,-2.557518616,3.3517750238  C 0.1945961239,-2.9018486715,-1.2160603411  C 0.1945961241,-2.9018486716,1.2160603416  H -0.1081386117,-3.9588421162,-1.2316817519  H -0.1081386115,-3.9588421162,1.2316817525  H 1.2848723236,-2.8633723421,-1.1729054707  H 1.2848723238,-2.8633723421,1.1729054712  C -1.4823673786,0.3562473176,-3.1520736001  C -1.4823673782,0.3562473175,3.152073601  H -2.3066807841,-0.1876969275,-2.6698114707  H -2.3066807837,-0.1876969276,2.6698114717  C -1.5096309562,0.0390058052,-4.6489904404  C -1.5096309556,0.039005805,4.6489904412  H -0.7002342046,0.5790642673,-5.1533303095  H -0.7002342039,0.5790642671,5.1533303103  H -1.334363274,-1.0265615352,-4.8277693331  H -1.3343632734,-1.0265615353,4.8277693339  C -2.841035896,0.4574708083,-5.27543304  C -2.8410358953,0.4574708082,5.2754330411  H -2.8303128488,0.2481544473,-6.3500336932  H -2.830312848,0.2481544472,6.3500336943  H -3.6466758767,-0.1516835271,-4.8469082453  H -3.6466758761,-0.1516835272,4.8469082465  C -3.1372259989,1.933725797,-5.0238215848  C -3.1372259982,1.9337257969,5.023821586  H -2.3971956431,2.5441585585,-5.5567065145  H -2.3971956424,2.5441585584,5.5567065155  H -4.1147497309,2.2000009506,-5.4380419964  H -4.1147497302,2.2000009504,5.4380419977  C -3.0810825806,2.2642169303,-3.5342752117  C -3.0810825801,2.2642169302,3.5342752129  H -3.8981991703,1.7462584044,-3.0167867814  H -3.8981991698,1.7462584043,3.0167867827  H -3.2431379179,3.334872578,-3.3759258562  H -3.2431379175,3.3348725779,3.3759258574  C -1.7508203467,1.8434501672,-2.9089332691  C -1.7508203463,1.8434501672,2.90893327</p>	<p>Fe-Cyclohexyl-2H-CO-TS</p> <p>H -1.8247206873,0.8903529952,0.  Fe -0.2272317513,0.4129667332,0.  N -0.0539255793,2.4888660767,0.  H 1.2689099138,0.1523134531,0.  C -0.4422428051,-1.309845676,0.  H -1.299981839,1.6915587896,0.  P -0.1218487469,0.6141150494,-2.2123367074  P -0.1218487469,0.6141150494,2.2123367074  O -0.5282942932,-2.4643921491,0.  C -0.069493671,2.4599494369,2.4437021229  C -0.069493671,2.4599494369,-2.4437021229  H -1.1073416762,2.7850560583,2.5611097782  H -1.1073416762,2.7850560583,-2.5611097782  H 0.476376484,2.7604299103,3.3407086337  H 0.476376484,2.7604299103,-3.3407086337  C 0.5241195195,3.0708078471,1.1862787888  C 0.5241195195,3.0708078471,-1.1862787888  H 0.3566256304,4.1616828416,1.202571443  H 0.3566256304,4.1616828416,-1.202571443  H 1.6208608727,2.9296791211,1.1971957712  H 1.6208608727,2.9296791211,-1.1971957712  C -1.6528925652,0.1920366482,3.2235245766  C -1.6528925652,0.1920366482,-3.2235245766  H -2.3937732722,0.8433503655,2.7381897788  H -2.3937732722,0.8433503655,-2.7381897788  C -1.5861934596,0.5806565065,4.7036119574  C -1.5861934596,0.5806565065,-4.7036119574  H -0.86062937,-0.0601123771,5.2178033104  H -0.86062937,-0.0601123771,-5.2178033104  H -1.2367696702,1.610277388,4.82187416  H -1.2367696702,1.610277388,-4.82187416  C -2.9501459423,0.4157648453,5.3768815217  C -2.9501459423,0.4157648453,-5.3768815217  H -2.8744400812,0.6728083984,6.4382523863  H -2.8744400812,0.6728083984,-6.4382523863  H -3.6566887719,1.1282605099,4.9334888062  H -3.6566887719,1.1282605099,-4.9334888062  C -3.4909573017,-1.001657621,5.2100384505  C -3.4909573017,-1.001657621,-5.2100384505  H -2.8475423966,-1.699132314,5.7610771685  H -2.8475423966,-1.699132314,-5.7610771685  H -4.487833873,-1.0821760744,5.6543785826  H -4.487833873,-1.0821760744,-5.6543785826  C -3.5284309523,-1.4095910503,3.739487307  C -3.5284309523,-1.4095910503,-3.739487307  H -4.2642295551,-0.7916663643,3.2098942779  H -4.2642295551,-0.7916663643,-3.2098942779  H -3.8649734721,-2.4461047548,3.6401294454  H -3.8649734721,-2.4461047548,-3.6401294454  C -2.1633053364,-1.2427036641,3.0711151597  C -2.1633053364,-1.2427036641,-3.0711151597</p>

<p>H -0.9477820517,2.4472678503,-3.3455864503  H -0.9477820512,2.4472678502,3.3455864512  H -1.7545159418,2.0452013628,-1.8365029049  H -1.7545159415,2.0452013628,1.8365029059  C 1.4881698023,0.0150065116,-3.2576134767  C 1.4881698027,0.0150065115,3.2576134772  H 1.17519687,-0.1276607145,-4.299522981  H 1.1751968706,-0.1276607146,4.2995229816  C 2.640504258,-0.9527845745,-2.968526053  C 2.6405042584,-0.9527845746,2.9685260533  H 2.8996073847,-0.8772812325,-1.9066784411  H 2.899607385,-0.8772812325,1.9066784414  H 2.3304403338,-1.9865781745,-3.1481899105  H 2.3304403342,-1.9865781745,3.1481899108  C 3.867666484,-0.6455312228,-3.8279543937  C 3.8676664845,-0.6455312229,3.8279543938  H 4.6772646461,-1.3370473477,-3.5727300978  H 4.6772646466,-1.3370473478,3.5727300978  H 3.6263509706,-0.8260613012,-4.8834423567  H 3.6263509713,-0.8260613013,4.8834423569  C 4.328727973,0.7984775763,-3.659309654  C 4.3287279735,0.7984775762,3.6593096542  H 5.1791946763,1.0060700608,-4.3164570275  H 5.1791946768,1.0060700607,4.3164570275  H 4.6823430079,0.9469562291,-2.6318498395  H 4.6823430082,0.9469562292,2.6318498396  C 3.1865859184,1.7694263643,-3.9409128831  C 3.186585919,1.7694263642,3.9409128834  H 2.9099550177,1.7058356358,-5.0011649723  H 2.9099550184,1.7058356356,5.0011649726  H 3.5098863297,2.8001525557,-3.7653093606  H 3.5098863302,2.8001525556,3.7653093609  C 1.9647807837,1.4606612269,-3.0759951811  C 1.9647807841,1.4606612268,3.0759951816  H 1.1629874732,2.166299126,-3.3055282875  H 1.1629874736,2.1662991259,3.3055282881  H 2.2172089189,1.6137779184,-2.021960519  H 2.2172089192,1.6137779183,2.0219605195</p>	<p>H -1.4575848088,-1.9412001493,3.5336070702  H -1.4575848088,-1.9412001493,-3.5336070702  H -2.2265362318,-1.5116758125,2.0156786562  H -2.2265362318,-1.5116758125,-2.0156786562  C 1.3381105481,-0.05877977,3.1763820634  C 1.3381105481,-0.05877977,-3.1763820634  H 1.1002072021,0.0940915878,4.2366327492  H 1.1002072021,0.0940915878,-4.2366327492  C 2.6330995912,0.7001123601,2.8654799497  C 2.6330995912,0.7001123601,-2.8654799497  H 2.8378490826,0.6206759344,1.792272273  H 2.8378490826,0.6206759344,-1.792272273  H 2.5195198837,1.7645359427,3.0865038862  H 2.5195198837,1.7645359427,-3.0865038862  C 3.8151913155,0.1429949617,3.6594040676  C 3.8151913155,0.1429949617,-3.6594040676  H 4.725325622,0.6902673513,3.3941477555  H 4.725325622,0.6902673513,-3.3941477555  H 3.6476959073,0.3190266896,4.7297464225  H 3.6476959073,0.3190266896,-4.7297464225  C 4.003390145,-1.3514439561,3.4202243347  C 4.003390145,-1.3514439561,-3.4202243347  H 4.8264396591,-1.7350315041,4.0312939234  H 4.8264396591,-1.7350315041,-4.0312939234  H 4.2863199632,-1.5168564574,2.3735707753  H 4.2863199632,-1.5168564574,-2.3735707753  C 2.7170709256,-2.1152613166,3.7179797491  C 2.7170709256,-2.1152613166,-3.7179797491  H 2.4972597079,-2.0502901574,4.7913092663  H 2.4972597079,-2.0502901574,-4.7913092663  H 2.8425274015,-3.1784202879,3.4907109854  H 2.8425274015,-3.1784202879,-3.4907109854  C 1.5371369149,-1.5575196137,2.922086872  C 1.5371369149,-1.5575196137,-2.922086872  H 0.6319875148,-2.1191302302,3.1638973357  H 0.6319875148,-2.1191302302,-3.1638973357  H 1.7161763926,-1.705640784,1.8521874689  H 1.7161763926,-1.705640784,-1.8521874689</p>
<p>Fe-Cyclohexyl-H-CO-16E</p> <p>N -0.1222454351,-2.0546033783,0.  Fe -0.3805702773,-0.2116198286,0.  P -0.170448195,-0.3412220394,2.2029391105  P -0.170448195,-0.3412220394,-2.2029391105  C -1.5703347695,1.0387005273,0.  O -2.4178923993,1.8346869882,0.  H 0.622677528,0.8939168412,0.  C -0.3805578149,-2.1699794533,-2.4479814293  C -0.3805578149,-2.1699794533,2.4479814293  H -1.4583734896,-2.3197548319,-2.5589434158  H -1.4583734896,-2.3197548319,2.5589434158  H 0.1038601534,-2.5551508612,-3.348570536  H 0.1038601534,-2.5551508612,3.348570536  C 0.1005255499,-2.8721223596,-1.187056869  C 0.1005255499,-2.8721223596,1.187056869  H -0.4293991753,-3.8324746816,-1.0847907974  H -0.4293991753,-3.8324746816,1.0847907974</p>	<p>Fe-Cyclohexyl-2H-CO-NCCH3-TS.out</p> <p>H,0,-1.3440647796,-2.5505147064,0.  H,0,-1.962908615,-0.5723481752,0.  N,0,-2.6742794806,-2.5654308559,0.  C,0,-2.8878853575,-1.3580023893,0.  C,0,-4.1618075873,-0.5671456313,0.  H,0,-5.0201401882,-1.2394058012,0.  H,0,-4.2074537904,0.0836917069,-0.8779791773  H,0,-4.2074537904,0.0836917069,0.8779791773  H,0,1.3067000328,-0.1140139692,0.  N,0,-0.1189697824,-2.2751598127,0.  Fe,0,-0.1793810589,-0.2627216056,0.  P,0,-0.0332659225,-0.449447601,2.2177035832  P,0,-0.0332659225,-0.449447601,-2.2177035832  C,0,-0.3314187852,1.4645932534,0.  O,0,-0.3903685153,2.6227168207,0.  C,0,-0.1050174906,-2.291283631,-2.4538294436  C,0,-0.1050174906,-2.291283631,2.4538294436</p>

H 1.1671089798,-3.132572468,-1.2818622573	H,0,-1.1610203773,-2.543387778,-2.5825297713
H 1.1671089798,-3.132572468,1.2818622573	H,0,-1.1610203773,-2.543387778,2.5825297713
C -1.4818079527,0.3630812017,-3.3495317901	H,0,0.4308093489,-2.6321145467,-3.3422360247
C -1.4818079527,0.3630812017,3.3495317901	H,0,0.4308093489,-2.6321145467,3.3422360247
H -2.40366782,0.0585489226,-2.8348301794	C,0,0.4212516162,-2.9450902624,-1.190580626
H -2.40366782,0.0585489226,2.8348301794	C,0,0.4212516162,-2.9450902624,1.190580626
C -1.5155225536,-0.2281327184,-4.7629681504	H,0,0.1390059009,-4.0084395687,-1.1795473169
C -1.5155225536,-0.2281327184,4.7629681504	H,0,0.1390059009,-4.0084395687,1.1795473169
H -0.6017605017,0.0509478263,-5.30138952	H,0,1.5164708466,-2.9069909366,-1.1660700893
H -0.6017605017,0.0509478263,5.30138952	H,0,1.5164708466,-2.9069909366,1.1660700893
H -1.5380293391,-1.320404039,-4.7291303931	C,0,-1.4540331042,0.0913091458,-3.3291622314
H -1.5380293391,-1.320404039,4.7291303931	C,0,-1.4540331042,0.0913091458,3.3291622314
C -2.7299920073,0.2832612705,-5.5426705998	H,0,-2.2959452656,-0.4304234045,-2.853089882
C -2.7299920073,0.2832612705,5.5426705998	H,0,-2.2959452656,-0.4304234045,2.853089882
H -2.7166445767,-0.1250769681,-6.5583116361	C,0,-1.3639968915,-0.3978296808,-4.7786730869
H -2.7166445767,-0.1250769681,6.5583116361	C,0,-1.3639968915,-0.3978296808,4.7786730869
H -3.6425259971,-0.096760914,-5.0670341011	H,0,-0.5279853987,0.100486473,-5.2834478995
H -3.6425259971,-0.096760914,5.0670341011	H,0,-0.5279853987,0.100486473,5.2834478995
C -2.7822902297,1.8085290947,-5.5830863367	H,0,-1.1607565692,-1.471210753,-4.8172355876
C -2.7822902297,1.8085290947,5.5830863367	H,0,-1.1607565692,-1.471210753,4.8172355876
H -1.9376940486,2.1825855945,-6.1756767932	C,0,-2.6524320427,-0.0919145543,-5.5451752026
H -1.9376940486,2.1825855945,6.1756767932	C,0,-2.6524320427,-0.0919145543,5.5451752026
H -3.6909041328,2.1417453187,-6.0941439887	H,0,-2.5542555341,-0.4267689401,-6.5826842412
H -3.6909041328,2.1417453187,6.0941439887	H,0,-2.5542555341,-0.4267689401,6.5826842412
C -2.7100619199,2.4026954912,-4.1794579849	H,0,-3.4749959308,-0.6710772711,-5.1080846062
C -2.7100619199,2.4026954912,4.1794579849	H,0,-3.4749959308,-0.6710772711,5.1080846062
H -3.613756123,2.136414655,-3.6185985664	C,0,-2.9967969057,1.3936208828,-5.4961831439
H -3.613756123,2.136414655,3.6185985664	C,0,-2.9967969057,1.3936208828,5.4961831439
H -2.6873515073,3.4956252936,-4.2298282843	H,0,-2.2325533311,1.9591735264,-6.0441179281
H -2.6873515073,3.4956252936,4.2298282843	H,0,-2.2325533311,1.9591735264,6.0441179281
C -1.4836224023,1.8937261844,-3.4235480325	H,0,-3.9464613833,1.5802519218,-6.0068975311
C -1.4836224023,1.8937261844,3.4235480325	H,0,-3.9464613833,1.5802519218,6.0068975311
H -0.5860385167,2.2293957656,-3.9546293207	C,0,-3.0584182689,1.8982997172,-4.057110537
H -0.5860385167,2.2293957656,3.9546293207	C,0,-3.0584182689,1.8982997172,4.057110537
H -1.4484863532,2.3311325667,-2.42445063	H,0,-3.9034464777,1.4236941209,-3.5431801807
H -1.4484863532,2.3311325667,2.42445063	H,0,-3.9034464777,1.4236941209,3.5431801807
C 1.4757858054,0.1026677189,-2.9999827005	H,0,-3.2498173486,2.9755481632,-4.0383219507
C 1.4757858054,0.1026677189,2.9999827005	H,0,-3.2498173486,2.9755481632,4.0383219507
H 1.3080234982,0.0715192014,-4.0847831211	C,0,-1.7693466223,1.5895076242,-3.2938877584
H 1.3080234982,0.0715192014,4.0847831211	C,0,-1.7693466223,1.5895076242,3.2938877584
C 2.5657329602,-0.9188901189,-2.654021171	H,0,-0.9485281406,2.1498707501,-3.7550232971
C 2.5657329602,-0.9188901189,2.654021171	H,0,-0.9485281406,2.1498707501,3.7550232971
H 2.6854254436,-0.9494274681,-1.5646105201	H,0,-1.8494566635,1.9424889235,-2.2639379374
H 2.6854254436,-0.9494274681,1.5646105201	H,0,-1.8494566635,1.9424889235,2.2639379374
H 2.2670762836,-1.9219920152,-2.9673260338	C,0,1.5302103987,0.1106418756,-3.0938965225
H 2.2670762836,-1.9219920152,2.9673260338	C,0,1.5302103987,0.1106418756,3.0938965225
C 3.9020003434,-0.5664425043,-3.3084590151	H,0,1.3198661726,0.0270965778,-4.1675605645
C 3.9020003434,-0.5664425043,3.3084590151	H,0,1.3198661726,0.0270965778,4.1675605645
H 4.6596445595,-1.3002608114,-3.0152724687	C,0,2.7328737007,-0.7843834507,-2.7759556013
H 4.6596445595,-1.3002608114,3.0152724687	C,0,2.7328737007,-0.7843834507,2.7759556013
H 3.8000329101,-0.6450684538,-4.3983872556	H,0,2.9152909001,-0.7579049039,-1.6956442414
H 3.8000329101,-0.6450684538,4.3983872556	H,0,2.9152909001,-0.7579049039,1.6956442414
C 4.357562913,0.8434474771,-2.9477524816	H,0,2.5214511684,-1.8240700077,-3.0384155872
C 4.357562913,0.8434474771,2.9477524816	H,0,2.5214511684,-1.8240700077,3.0384155872
H 5.2887453471,1.0879926117,-3.4683586781	C,0,3.9871948721,-0.3201115617,-3.5178123607
H 5.2887453471,1.0879926117,3.4683586781	C,0,3.9871948721,-0.3201115617,3.5178123607
H 4.5777191066,0.8884257456,-1.8741363314	H,0,4.8317444762,-0.9626171206,-3.2491884276

<p>H 4.5777191066,0.8884257456,1.8741363314  C 3.2746188483,1.8649680689,-3.2791674907  C 3.2746188483,1.8649680689,3.2791674907  H 3.1388144866,1.9090393563,-4.3675346725  H 3.1388144866,1.9090393563,4.3675346725  H 3.5863003665,2.8662253569,-2.9655079748  H 3.5863003665,2.8662253569,2.9655079748  C 1.9461102258,1.5098088267,-2.6124145972  C 1.9461102258,1.5098088267,2.6124145972  H 1.1933974004,2.2583596199,-2.8652770698  H 1.1933974004,2.2583596199,2.8652770698  H 2.0542830758,1.5470069886,-1.5237534194  H 2.0542830758,1.5470069886,1.5237534194</p>	<p>H,0,4.8317444762,-0.9626171206,3.2491884276  H,0,3.8345884637,-0.4439951999,-4.5975016049  H,0,3.8345884637,-0.4439951999,4.5975016049  C,0,4.3135366614,1.1398842268,-3.2202178255  C,0,4.3135366614,1.1398842268,3.2202178255  H,0,5.1855498257,1.4601464081,-3.7989179737  H,0,5.1855498257,1.4601464081,3.7989179737  H,0,4.5861919136,1.2404655263,-2.1625385148  H,0,4.5861919136,1.2404655263,2.1625385148  C,0,3.1171209118,2.0387409022,-3.5157968365  C,0,3.1171209118,2.0387409022,3.5157968365  H,0,2.9193416534,2.0368244956,-4.5953278071  H,0,2.9193416534,2.0368244956,4.5953278071  H,0,3.3415724545,3.0745820926,-3.2433501245  H,0,3.3415724545,3.0745820926,3.2433501245  C,0,1.8688007477,1.5702086327,-2.7683409227  C,0,1.8688007477,1.5702086327,2.7683409227  H,0,1.0290611764,2.2282858867,-3.0004585609  H,0,1.0290611764,2.2282858867,3.0004585609  H,0,2.0363516303,1.6544835513,-1.6896824695  H,0,2.0363516303,1.6544835513,1.6896824695</p>
<p>Fe-Cyclohexyl-2H-CO-NC-Ph-TS.out</p> <p>H,0,-0.6823637181,-2.6126105811,0.  H,0,-1.4340138228,-0.6762357247,0.  N,0,-2.0169143711,-2.7098348642,0.  C,0,-2.2988726291,-1.5110136588,0.  C,0,-3.6121260541,-0.828667659,0.  H,0,1.8358558831,-0.0409782269,0.  N,0,0.518178596,-2.2767226726,0.  Fe,0,0.3621460083,-0.2699033021,0.  P,0,0.5122696278,-0.4513226343,2.2230228868  P,0,0.5122696278,-0.4513226343,-2.2230228868  C,0,0.1389453042,1.4488961528,0.  O,0,0.0350948002,2.6040297295,0.  C,0,0.5166386679,-2.2948010627,-2.4517269046  C,0,0.5166386679,-2.2948010627,2.4517269046  H,0,-0.5297328957,-2.5907719987,-2.5646627188  H,0,-0.5297328957,-2.5907719987,2.5646627188  H,0,1.0532117537,-2.6171924614,-3.3464406257  H,0,1.0532117537,-2.6171924614,3.3464406257  C,0,1.0855756379,-2.9205713082,-1.1927689431  C,0,1.0855756379,-2.9205713082,1.1927689431  H,0,0.8571340778,-3.9965627384,-1.1784474059  H,0,0.8571340778,-3.9965627384,1.1784474059  H,0,2.1772989306,-2.826433687,-1.1749532004  H,0,2.1772989306,-2.826433687,1.1749532004  C,0,-0.9287818634,0.0389804622,-3.328899129  C,0,-0.9287818634,0.0389804622,3.328899129  H,0,-1.7631354199,-0.4675150134,-2.8245109494  H,0,-1.7631354199,-0.4675150134,2.8245109494  C,0,-0.8562681638,-0.4949888311,-4.7635860732  C,0,-0.8562681638,-0.4949888311,4.7635860732  H,0,-0.0271963477,-0.0127072343,-5.2951154352  H,0,-0.0271963477,-0.0127072343,5.2951154352  H,0,-0.6531007788,-1.5688525597,-4.771008077  H,0,-0.6531007788,-1.5688525597,4.771008077</p>	

C,0,-2.1566448742,-0.214935739,-5.5203922421  
 C,0,-2.1566448742,-0.214935739,5.5203922421  
 H,0,-2.0721584647,-0.581471959,-6.5483871486  
 H,0,-2.0721584647,-0.581471959,6.5483871486  
 H,0,-2.9704432408,-0.7822128373,-5.0529906453  
 H,0,-2.9704432408,-0.7822128373,5.0529906453  
 C,0,-2.5062636266,1.2704230754,-5.5118731232  
 C,0,-2.5062636266,1.2704230754,5.5118731232  
 H,0,-1.7535182875,1.8215857114,-6.0898599218  
 H,0,-1.7535182875,1.8215857114,6.0898599218  
 H,0,-3.4649653965,1.436642916,-6.0126297214  
 H,0,-3.4649653965,1.436642916,6.0126297214  
 C,0,-2.5474984974,1.8189361331,-4.0884059826  
 C,0,-2.5474984974,1.8189361331,4.0884059826  
 H,0,-3.3800734224,1.3590498524,-3.5432428904  
 H,0,-3.3800734224,1.3590498524,3.5432428904  
 H,0,-2.7405651414,2.8960848277,-4.1010345536  
 H,0,-2.7405651414,2.8960848277,4.1010345536  
 C,0,-1.2442314353,1.537680511,-3.3397341515  
 C,0,-1.2442314353,1.537680511,3.3397341515  
 H,0,-0.4315139428,2.0795466496,-3.8363659471  
 H,0,-0.4315139428,2.0795466496,3.8363659471  
 H,0,-1.3059016522,1.9273415857,-2.3220530359  
 H,0,-1.3059016522,1.9273415857,2.3220530359  
 C,0,2.050707337,0.1768346113,-3.0971331761  
 C,0,2.050707337,0.1768346113,3.0971331761  
 H,0,1.8334791156,0.114031615,-4.171092236  
 H,0,1.8334791156,0.114031615,4.171092236  
 C,0,3.2841336044,-0.6869958158,-2.8114880267  
 C,0,3.2841336044,-0.6869958158,2.8114880267  
 H,0,3.4734636185,-0.6831717938,-1.7319310885  
 H,0,3.4734636185,-0.6831717938,1.7319310885  
 H,0,3.105702531,-1.7257590154,-3.1008161317  
 H,0,3.105702531,-1.7257590154,3.1008161317  
 C,0,4.5181351155,-0.1638899747,-3.5486246215  
 C,0,4.5181351155,-0.1638899747,3.5486246215  
 H,0,5.384204546,-0.7861721467,-3.3017833275  
 H,0,5.384204546,-0.7861721467,3.3017833275  
 H,0,4.3616002763,-0.2657047071,-4.6300373833  
 H,0,4.3616002763,-0.2657047071,4.6300373833  
 C,0,4.8005279781,1.2976886036,-3.2162800338  
 C,0,4.8005279781,1.2976886036,3.2162800338  
 H,0,5.6573219922,1.6598701348,-3.7929128646  
 H,0,5.6573219922,1.6598701348,3.7929128646  
 H,0,5.0781831734,1.3801865538,-2.1583282562  
 H,0,5.0781831734,1.3801865538,2.1583282562  
 C,0,3.5737612946,2.1645500049,-3.4802823489  
 C,0,3.5737612946,2.1645500049,3.4802823489  
 H,0,3.3677877526,2.1842295413,-4.5580761938  
 H,0,3.3677877526,2.1842295413,4.5580761938  
 H,0,3.766859553,3.1997742592,-3.1826863689  
 H,0,3.766859553,3.1997742592,3.1826863689  
 C,0,2.3468978168,1.637588508,-2.7362320539  
 C,0,2.3468978168,1.637588508,2.7362320539  
 H,0,1.4854570451,2.2754648612,-2.9433339581  
 H,0,1.4854570451,2.2754648612,2.9433339581  
 H,0,2.5210277953,1.6975133234,-1.6570267396

<p>H,0,2.5210277953,1.6975133234,1.6570267396  C,0,-3.69795497,0.5614097176,0.  C,0,-4.9362149687,1.1920581849,0.  C,0,-6.1002008424,0.434508451,0.  C,0,-4.7870765016,-1.5855801065,0.  C,0,-6.0211718916,-0.9562597436,0.  H,0,-2.7842206003,1.1473572826,0.  H,0,-4.9917338081,2.2752153552,0.  H,0,-7.0679876541,0.9241693358,0.  H,0,-4.7016993016,-2.6662823119,0.  H,0,-6.9292954917,-1.5495954082,0.</p>	
<p><b>Ph-CN</b></p> <p>N 0.0000000 0.0000000 3.1245589  C 0.0000000 0.0000000 1.9704733  C 0.0000000 0.0000000 0.5427256  C 1.2114708 0.0000000 -0.1553408  C -1.2114708 0.0000000 -0.1553408  C 1.2047734 0.0000000 -1.5411554  C -1.2047734 0.0000000 -1.5411554  C 0.0000000 0.0000000 -2.2346465  H 0.0000000 0.0000000 -3.3186581  H 2.1451381 0.0000000 0.3936460  H -2.1451381 0.0000000 0.3936460  H -2.1438881 0.0000000 -2.0820760  H 2.1438881 0.0000000 -2.0820760</p>	<p><b>Ph-CN=NH</b></p> <p>H -0.0035391 0.0000000 -3.7712006  N -0.4005379 0.0000000 -2.8332278  C 0.5143613 0.0000000 -1.9524542  H 1.5841584 0.0000000 -2.2039748  C 0.2267273 0.0000000 -0.5110282  C -0.2694147 0.0000000 2.2324811  C 1.2839485 0.0000000 0.3993330  C -1.0866753 0.0000000 -0.0329244  C -1.3304917 0.0000000 1.3298217  C 1.0386690 0.0000000 1.7659490  H 2.3056755 0.0000000 0.0312706  H -1.8986178 0.0000000 -0.7506495  H -2.3514376 0.0000000 1.6954349  H 1.8665496 0.0000000 2.4660103  H -0.4648195 0.0000000 3.2991885</p>
<p><b>MeCN</b></p> <p>C -0.0000001 0.0000000 1.0073347  N -0.0000001 0.0000000 2.1585001  C -0.0000001 0.0000000 -0.4432406  H 1.0243448 0.0000000 -0.8197509  H -0.5121726 0.8871087 -0.8197509  H -0.5121725 -0.8871087 -0.8197509</p>	<p><b>Me-CH=NH</b></p> <p>C 0.0557174 -0.0438872 1.0222972  H 0.3615015 0.8559734 1.5760909  H -0.1295686 0.9193847 -0.5911268  N -0.2268998 -0.0228700 -0.2118542  C -0.0060538 -1.3013211 1.8215999  H 0.9712360 -1.5222077 2.2626064  H -0.3164209 -2.1346476 1.1917213  H -0.7095125 -1.1914025 2.6531266</p>