

Iminium Substituent Drives Cyanide and Hydride Additions to Triiron Vinyliminium Complexes

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Supporting Information

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Figure S1. ^1H NMR spectrum (401 MHz, CDCl_3) of **2a**.

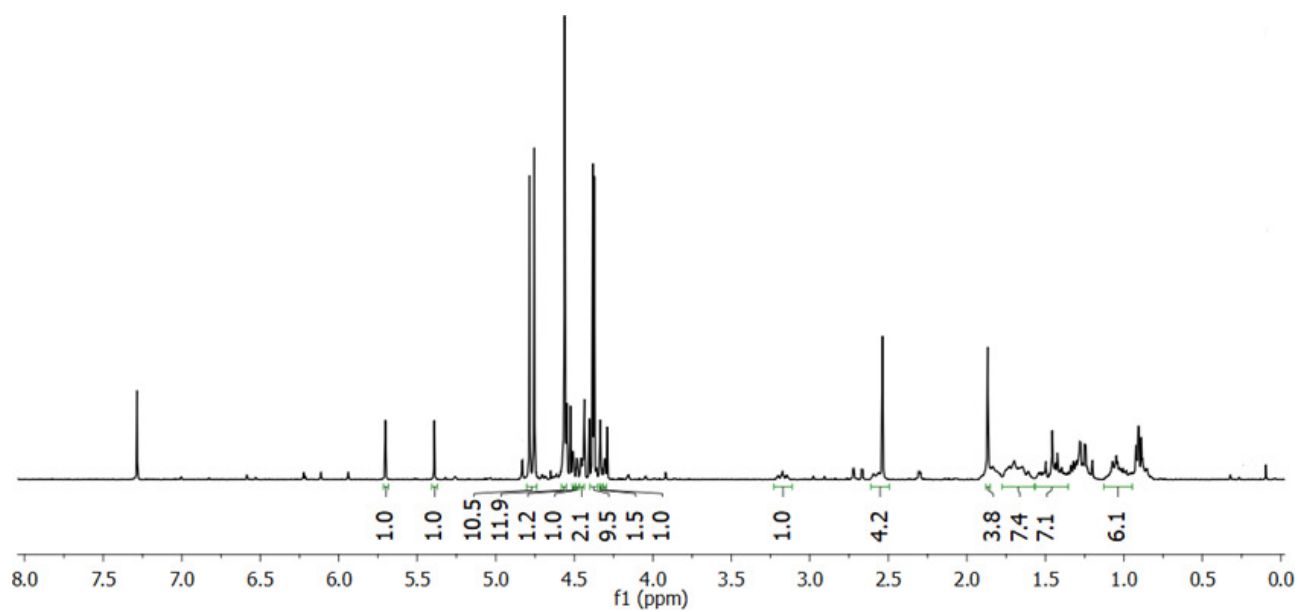


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **2a**.

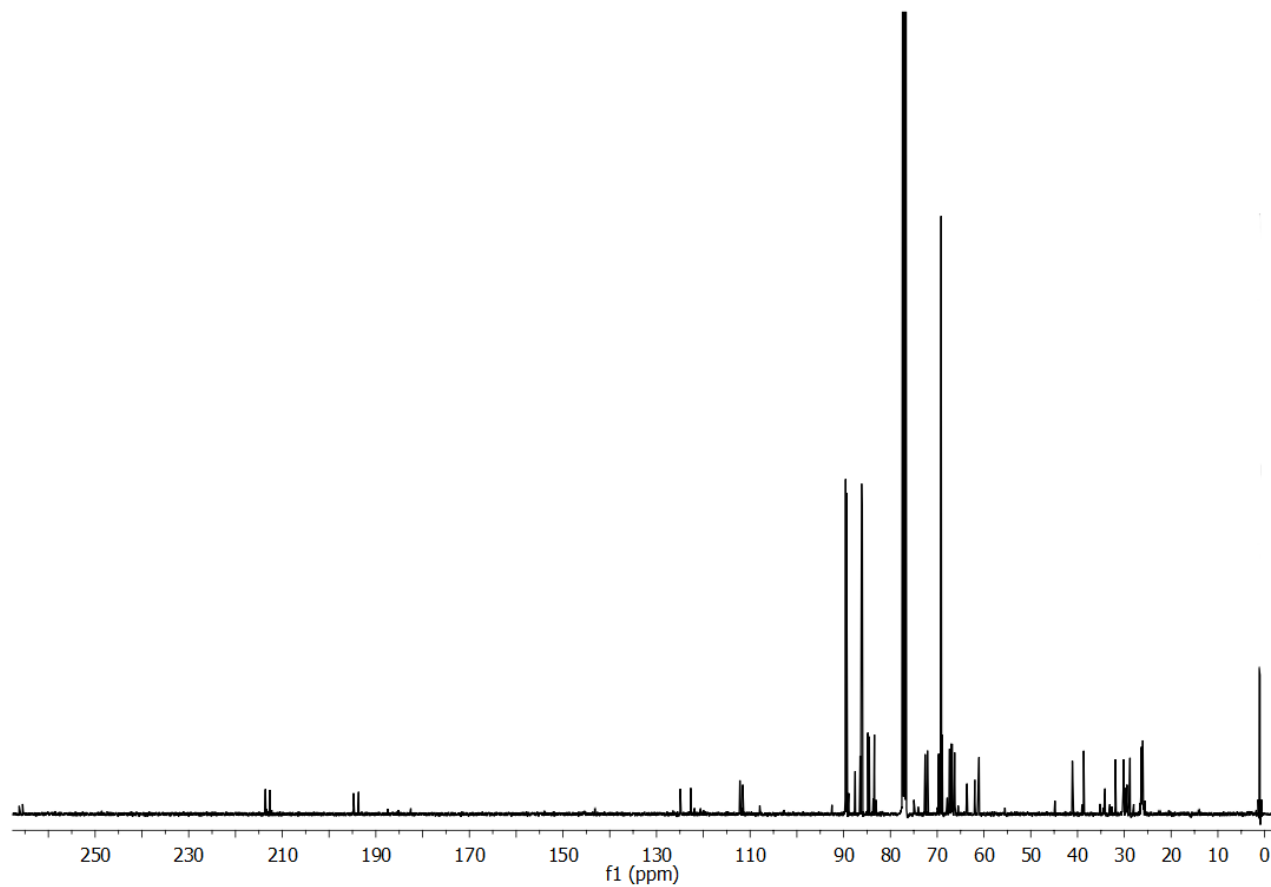


Figure S3. ^1H NMR spectrum (401 MHz, CDCl_3) of **2b**.

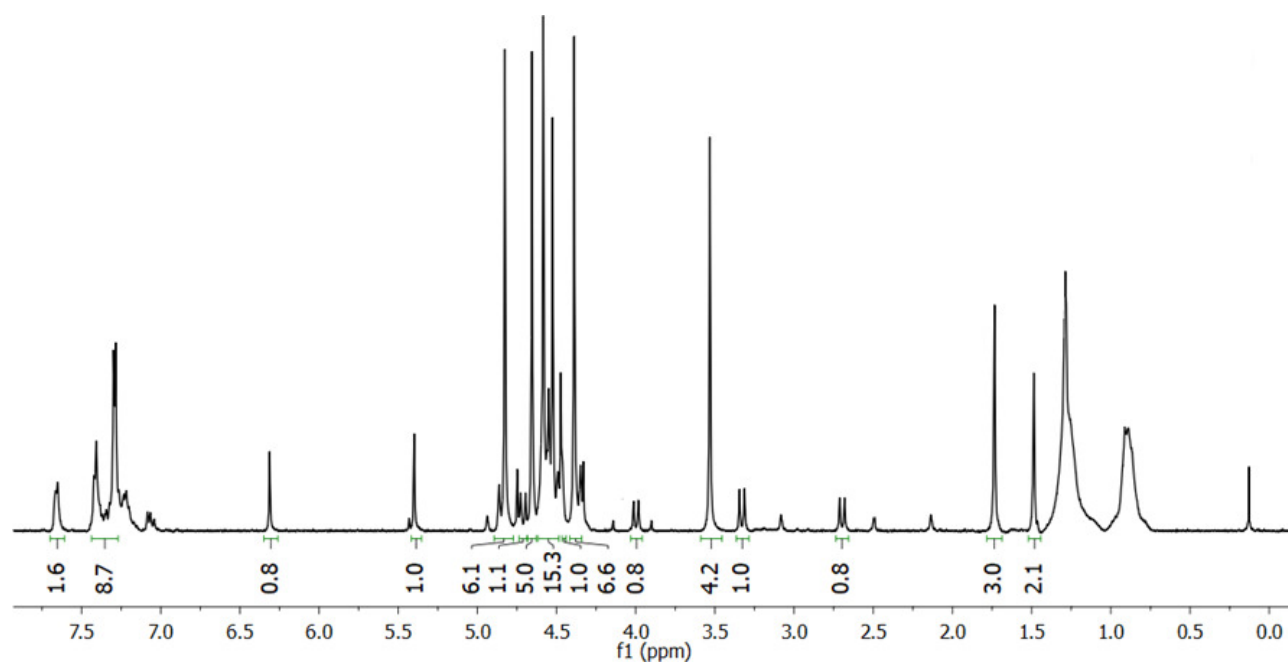


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **2b**.

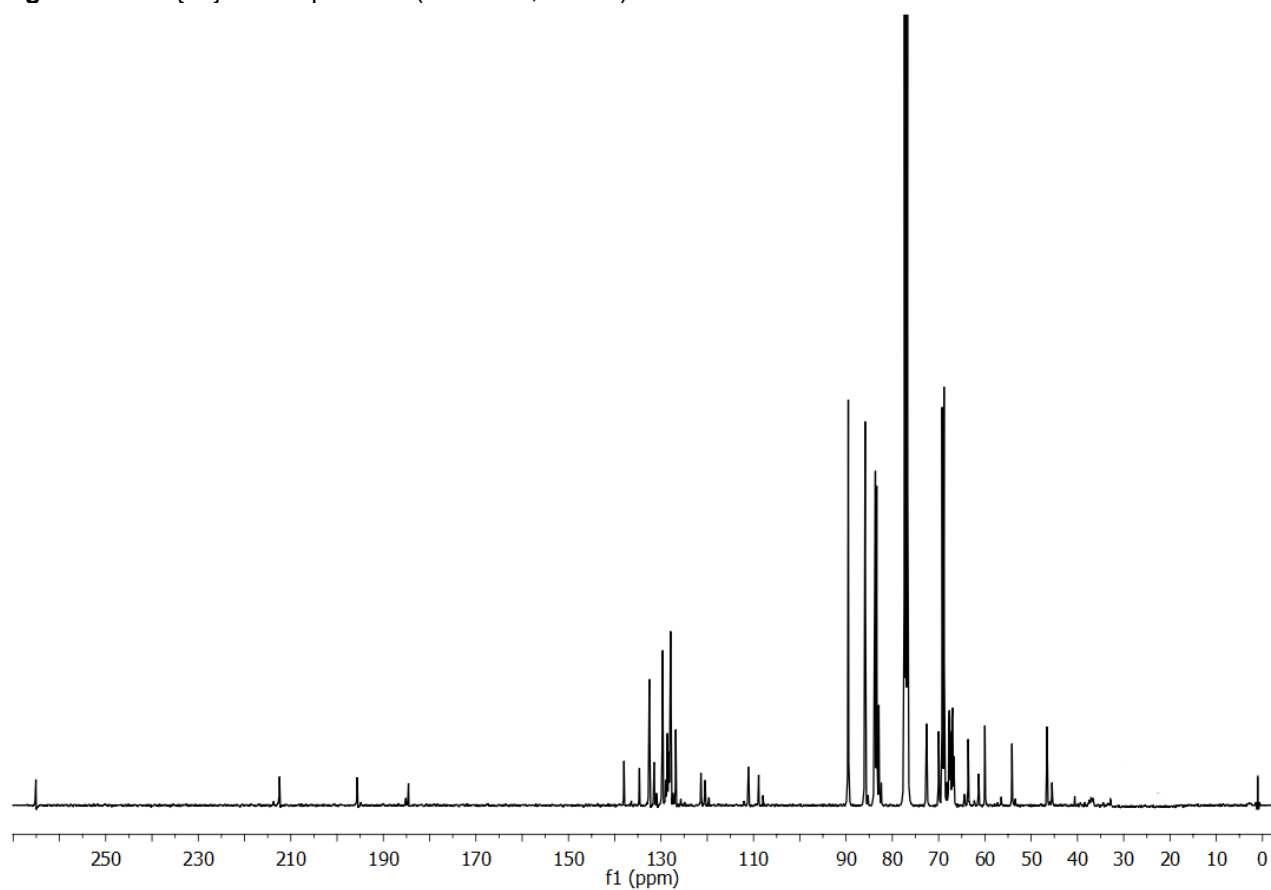


Figure S5. ^1H NMR spectrum (401 MHz, CDCl_3) of **2c**.

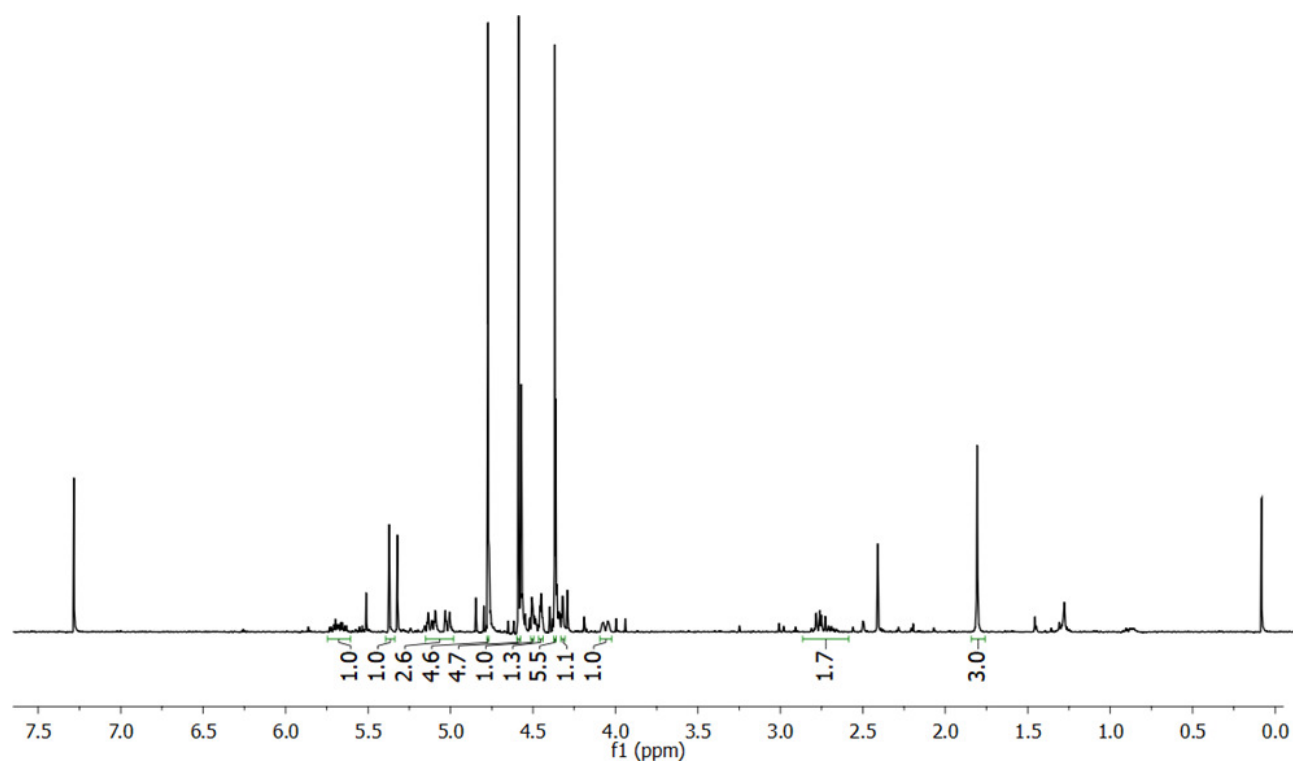


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **2c**.

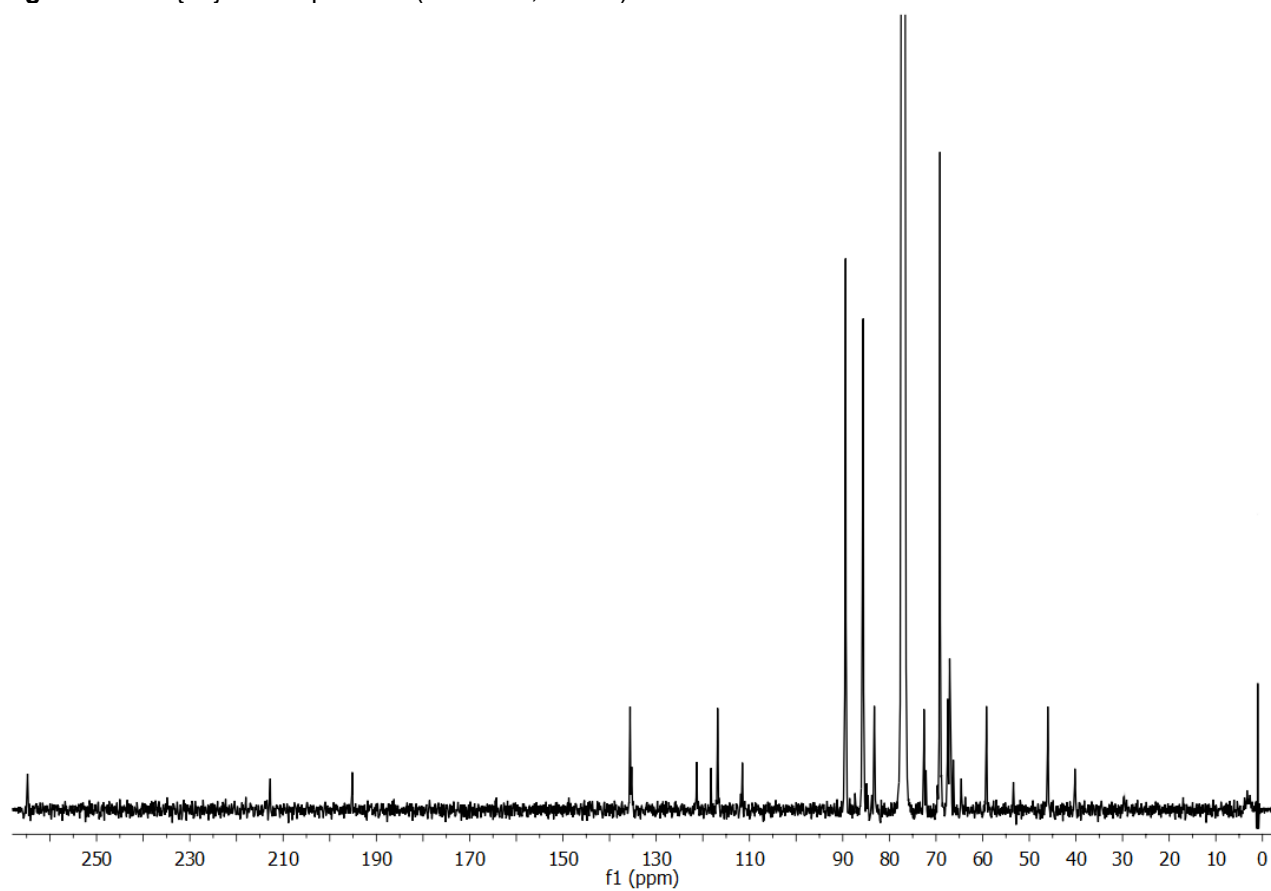


Figure S7. ^1H NMR spectrum (401 MHz, CDCl_3) of **2d/4d** mixture.

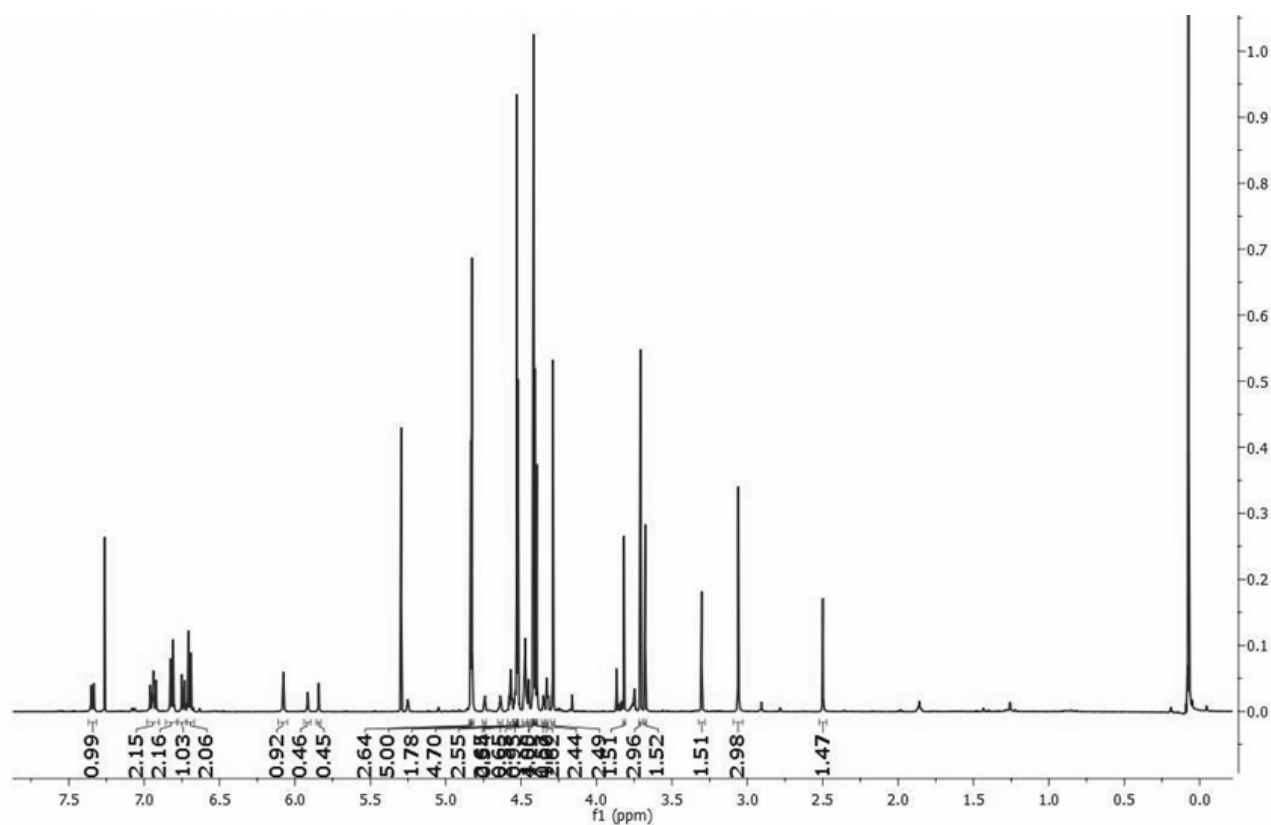


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **2d/4d** mixture.

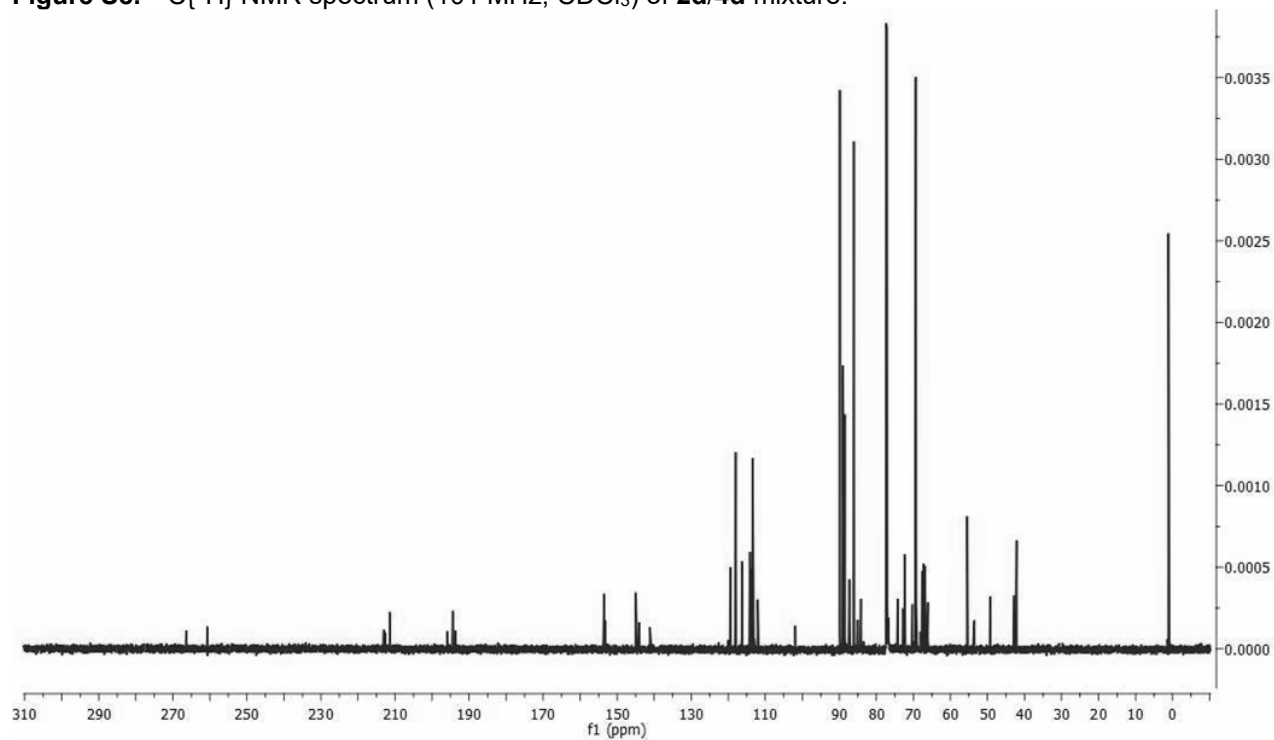


Figure S9. ^1H NMR spectrum (401 MHz, CDCl_3) of **4e**.

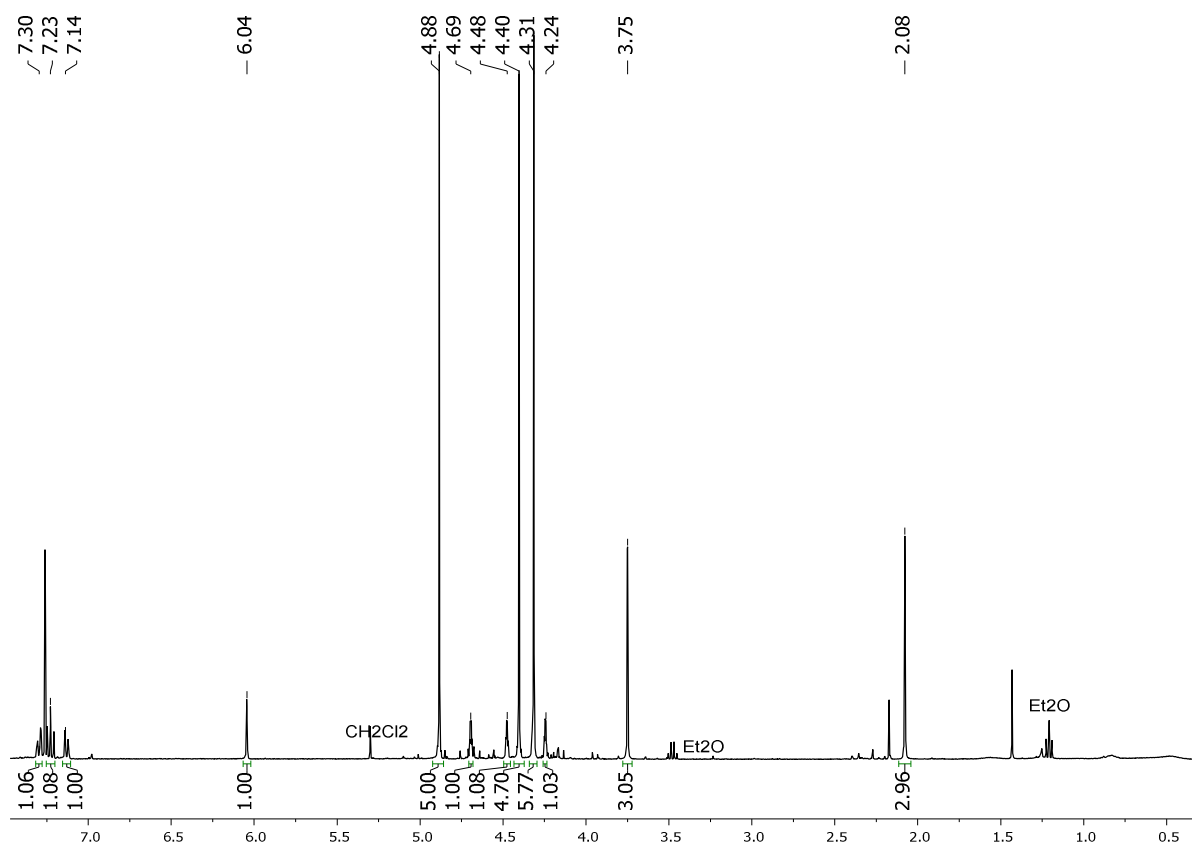


Figure S10. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **4e**.

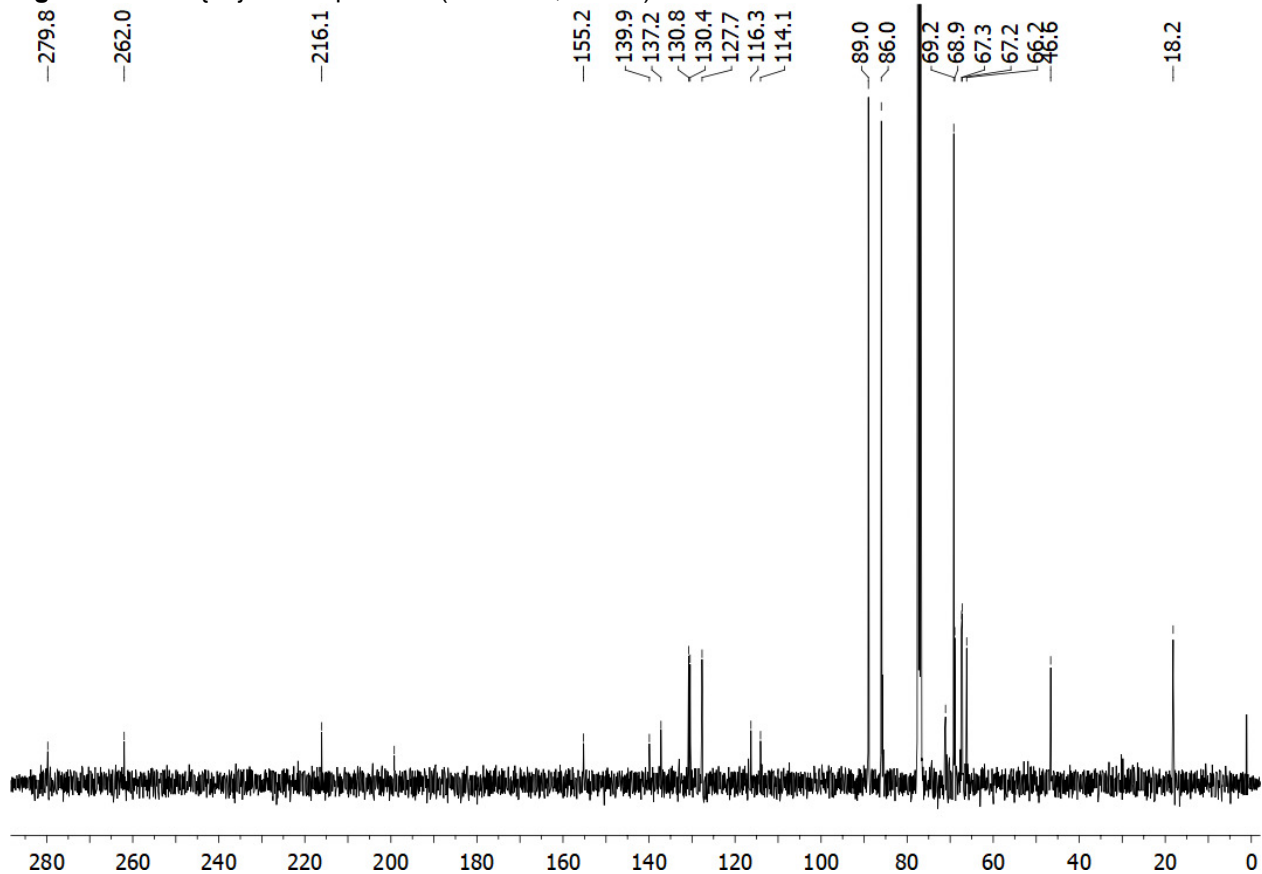


Figure S11. ^1H NMR spectrum (401 MHz, CDCl_3) of **5a**.

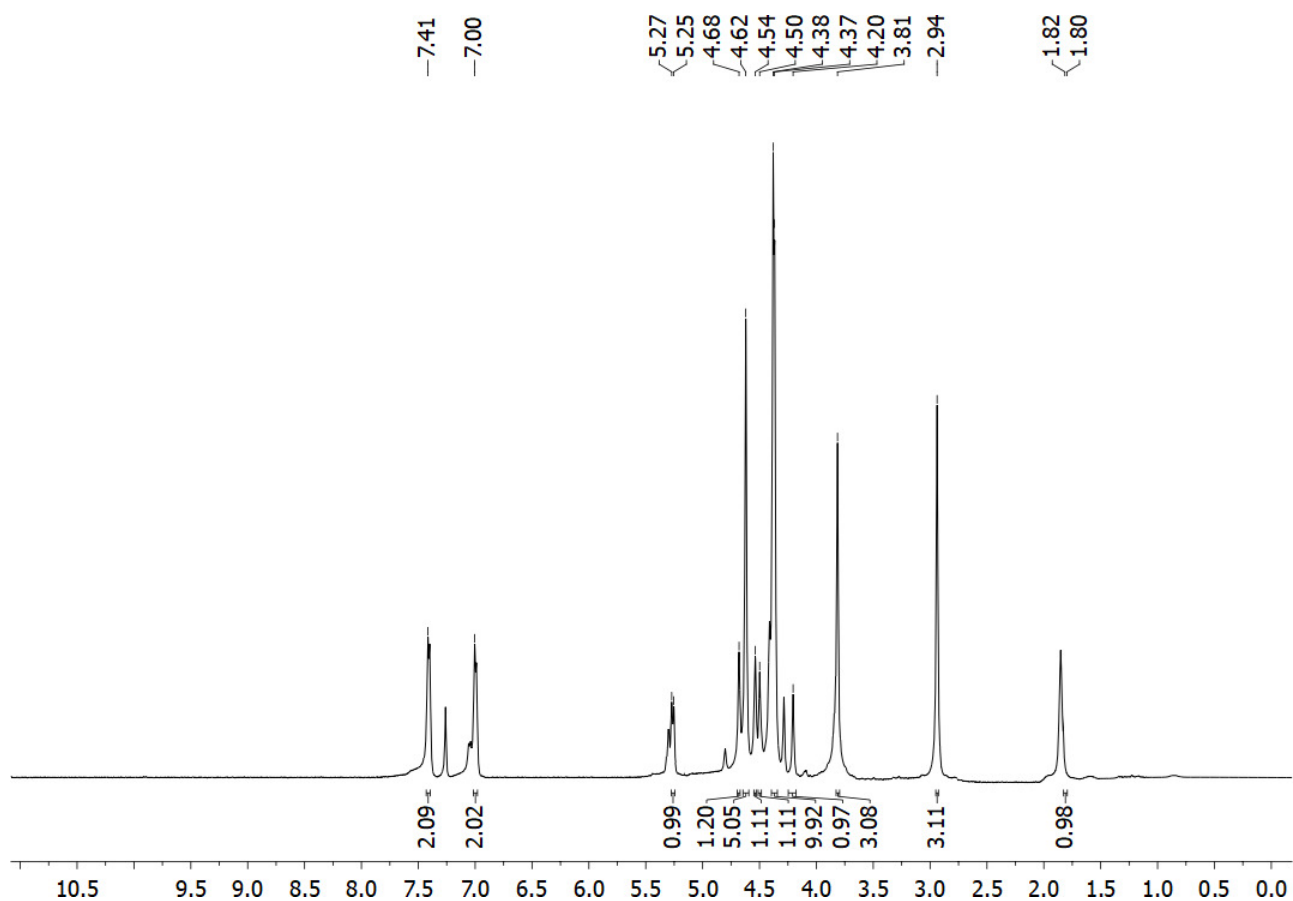


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **5a**.

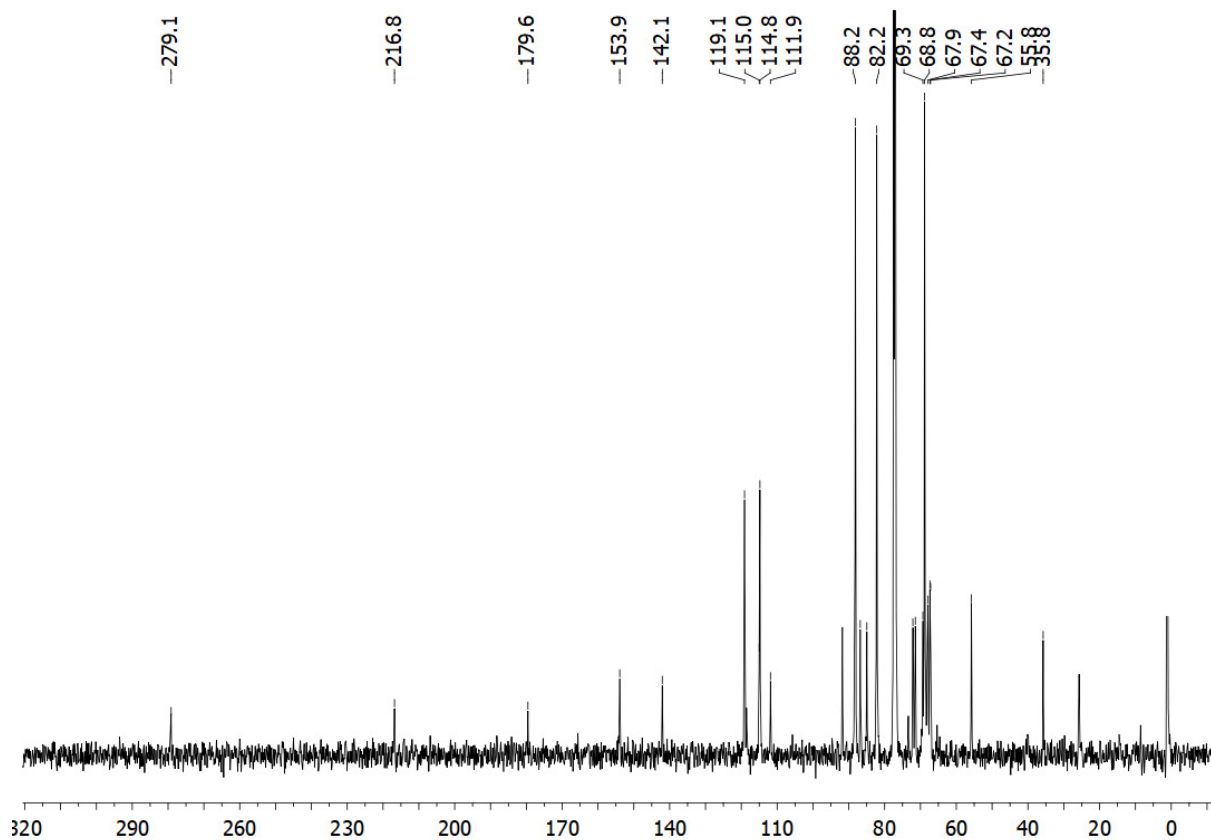


Figure S13. ^1H NMR spectrum (401 MHz, CDCl_3) of **6**.

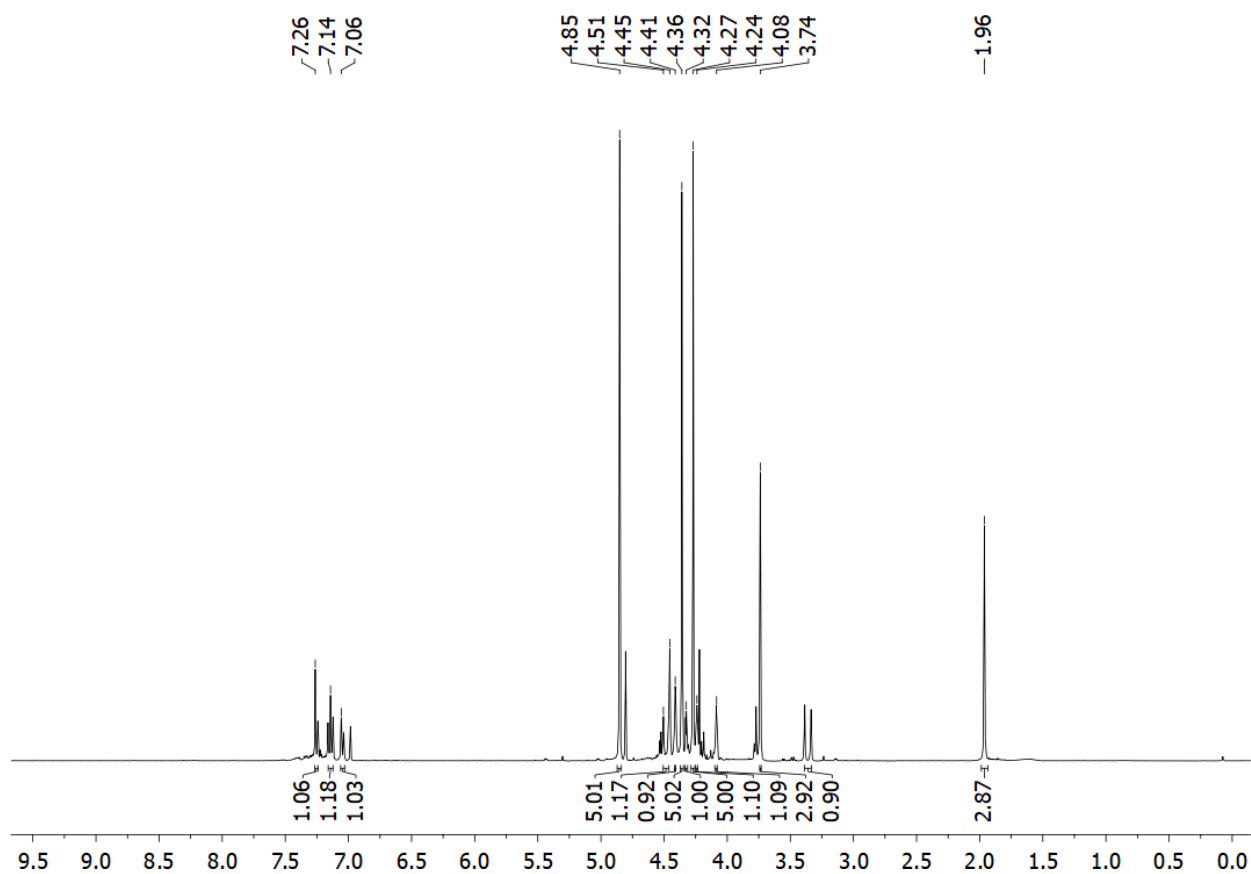


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **6**.

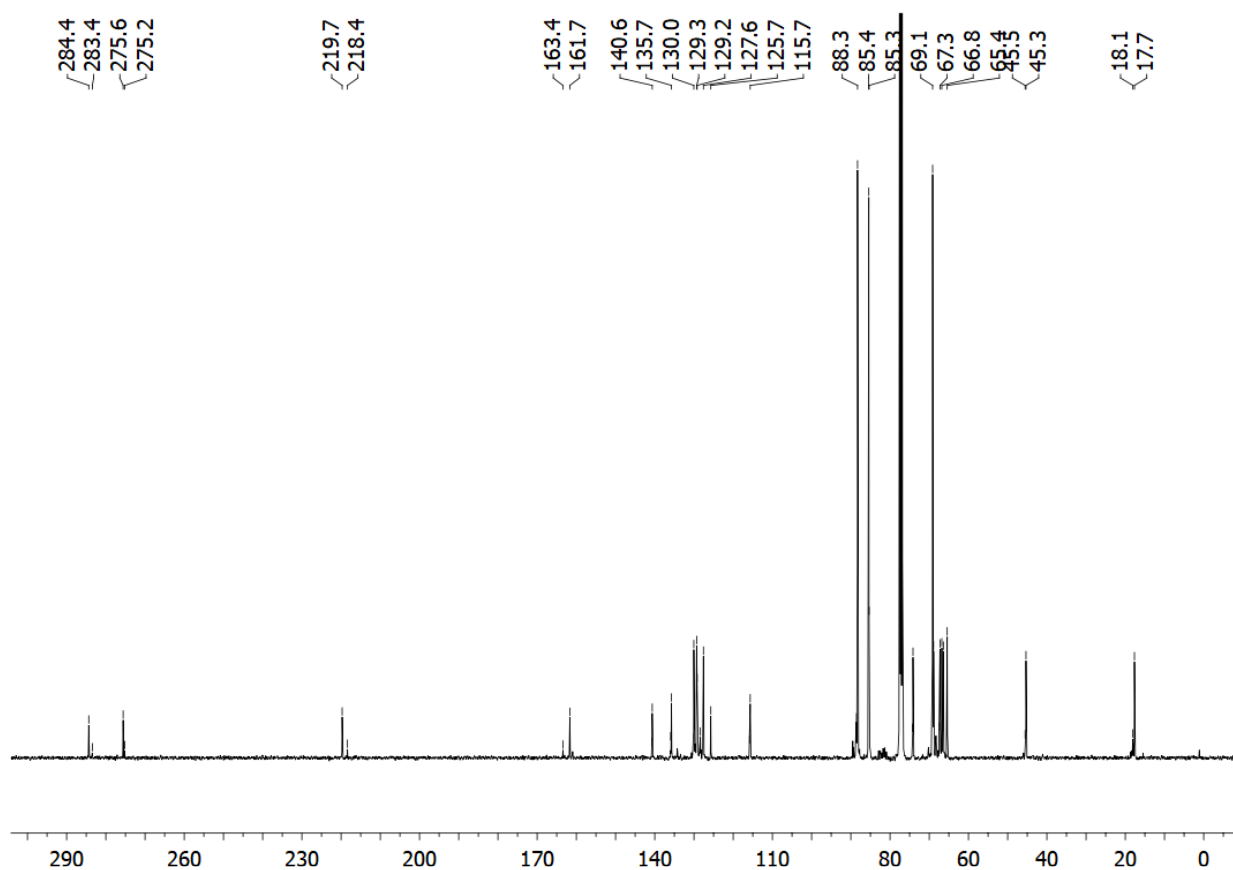


Figure S15. ^1H NMR spectrum (401 MHz, CDCl_3) of **2e**.

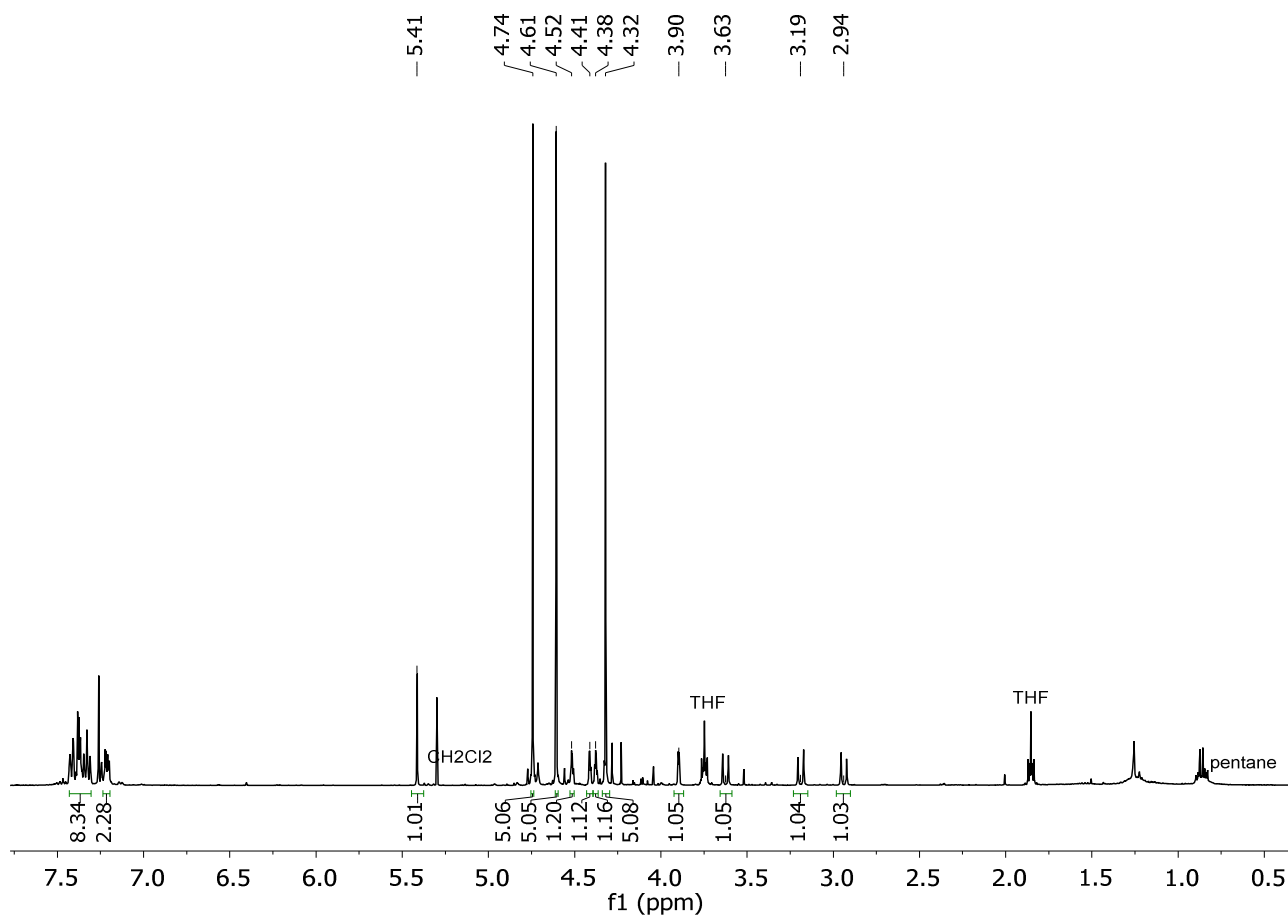


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **2e**.

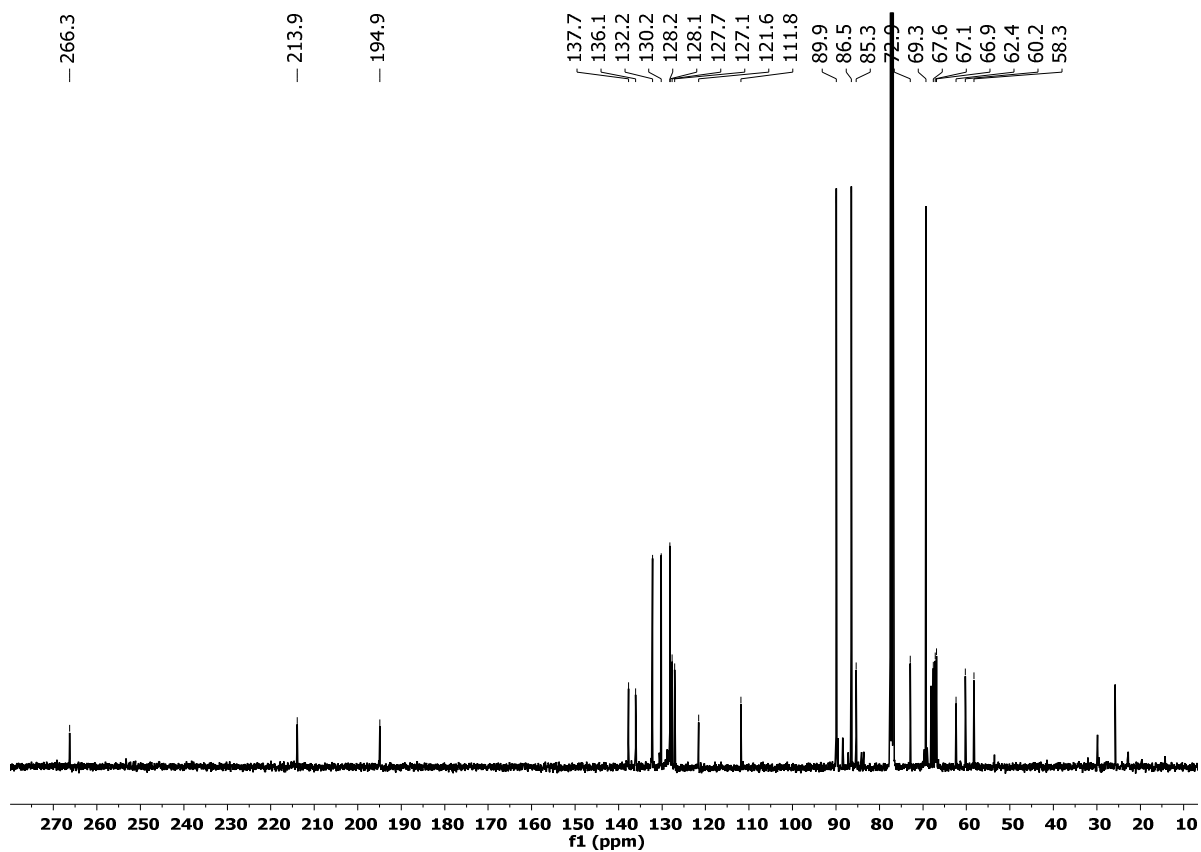


Figure S17. ^1H NMR spectrum (401 MHz, CDCl_3) of **5b**.

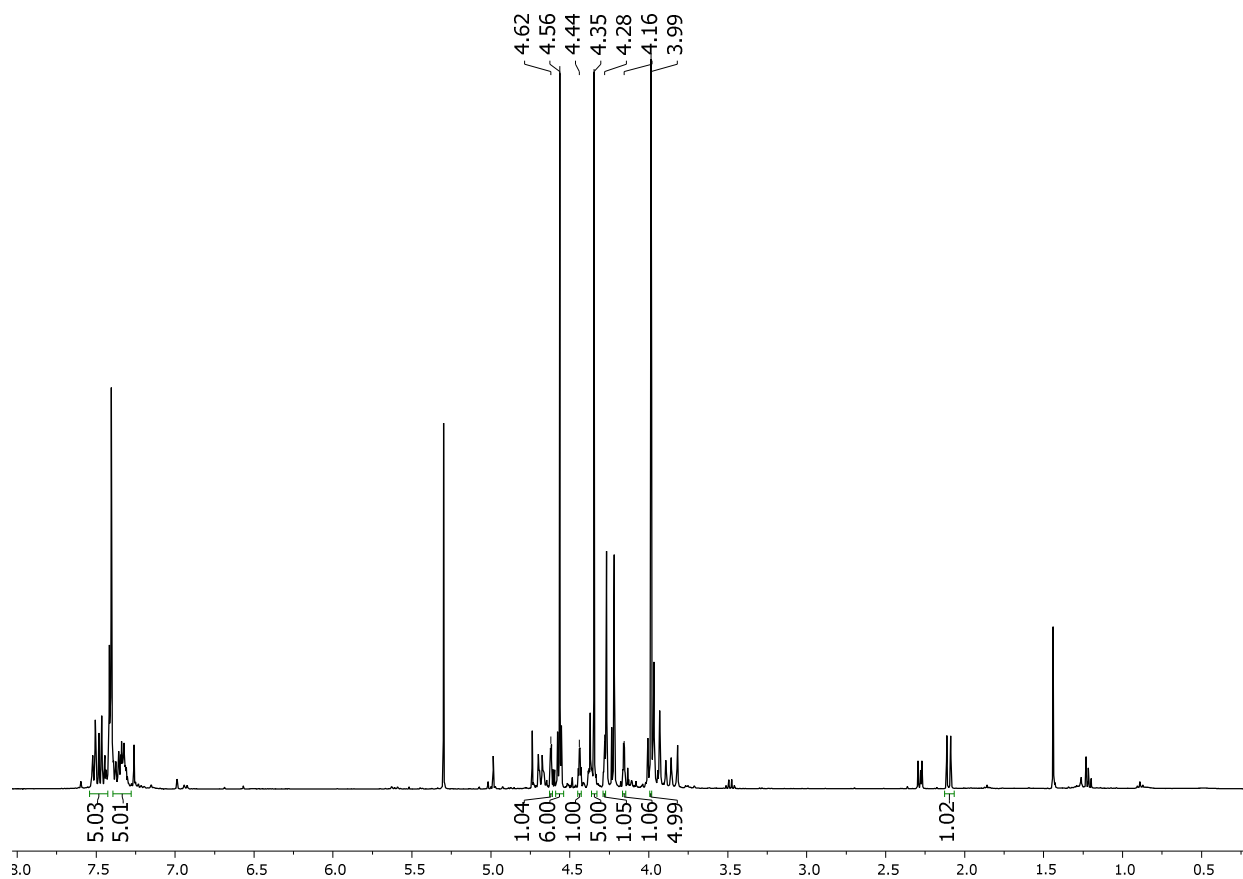


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **5b**.

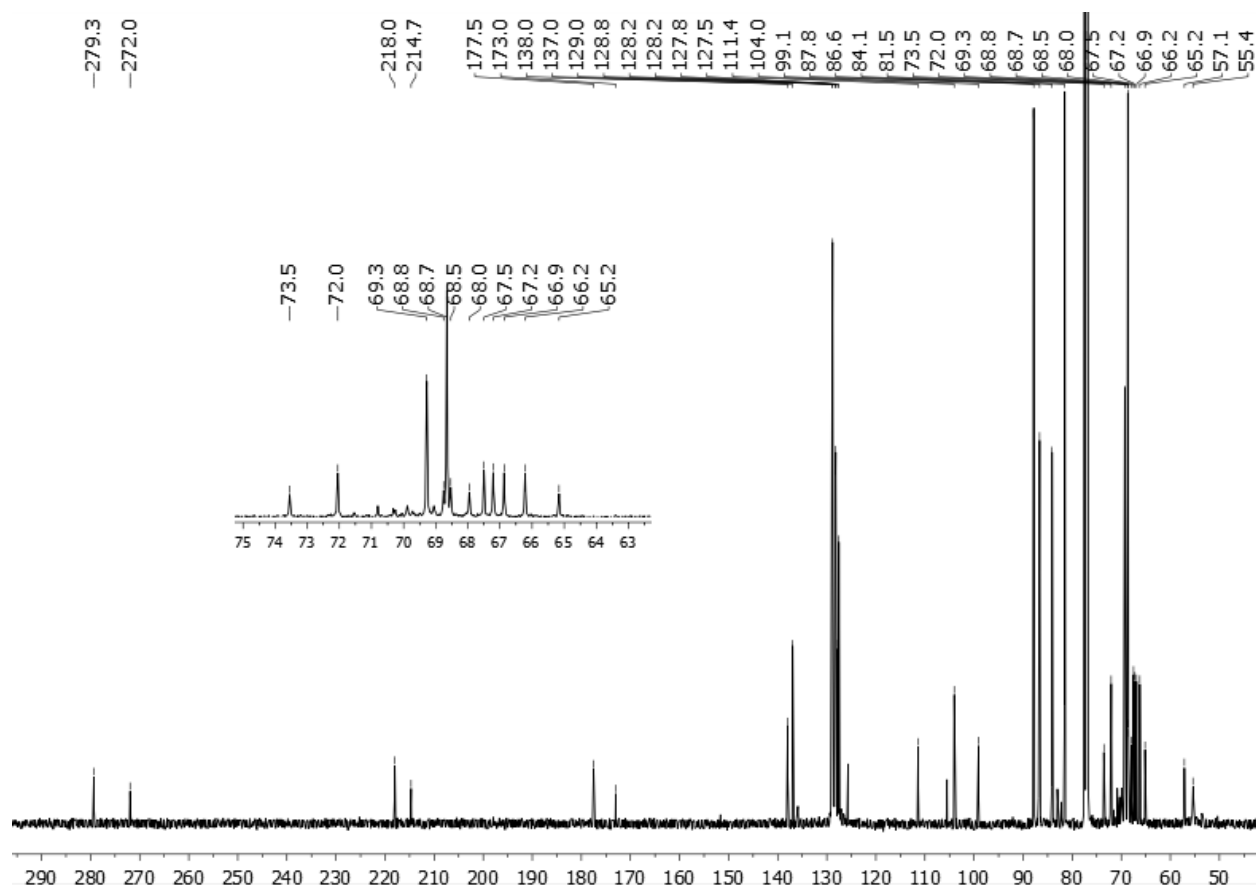


Figure S19. Relative Gibbs energy (kcal mol^{-1}) of products of cyanide addition to $[\mathbf{1c}]^+$. Black text, C^1 addition; blue text, C^2 addition. Hydrogen atoms, except $\text{C}^2\text{-H}$, have been omitted for clarity. Colour map: Fe, violet; N, blue; O, red; C, grey; H, white.

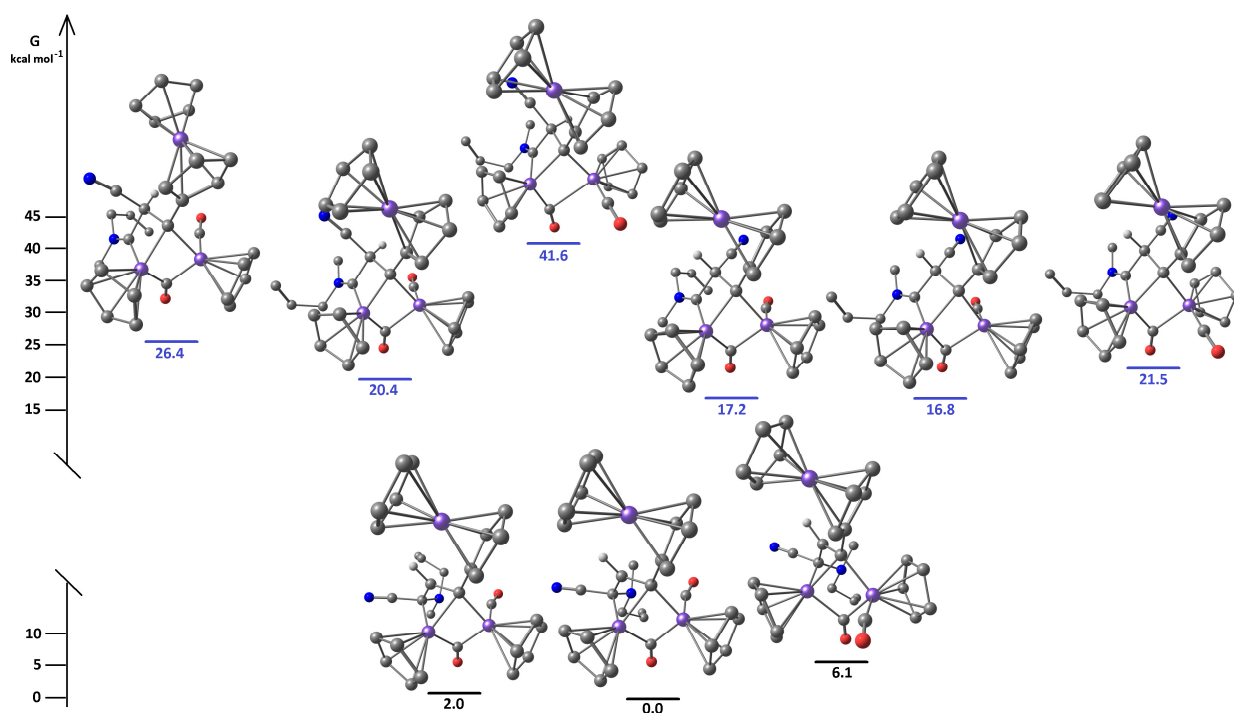


Figure S20. Relative energy variation (kcal mol^{-1}) on scanning the $\text{C}(\text{CN})\text{-C}^1\text{-N}^1\text{-C}^4$ dihedral angle of $\mathbf{2c}$ ($^\circ$, see main text, Figure 1). Hydrogen atoms, except $\text{C}^2\text{-H}$, have been omitted for clarity. Colour map: Fe, violet; N, blue; O, red; C, grey; H, white.

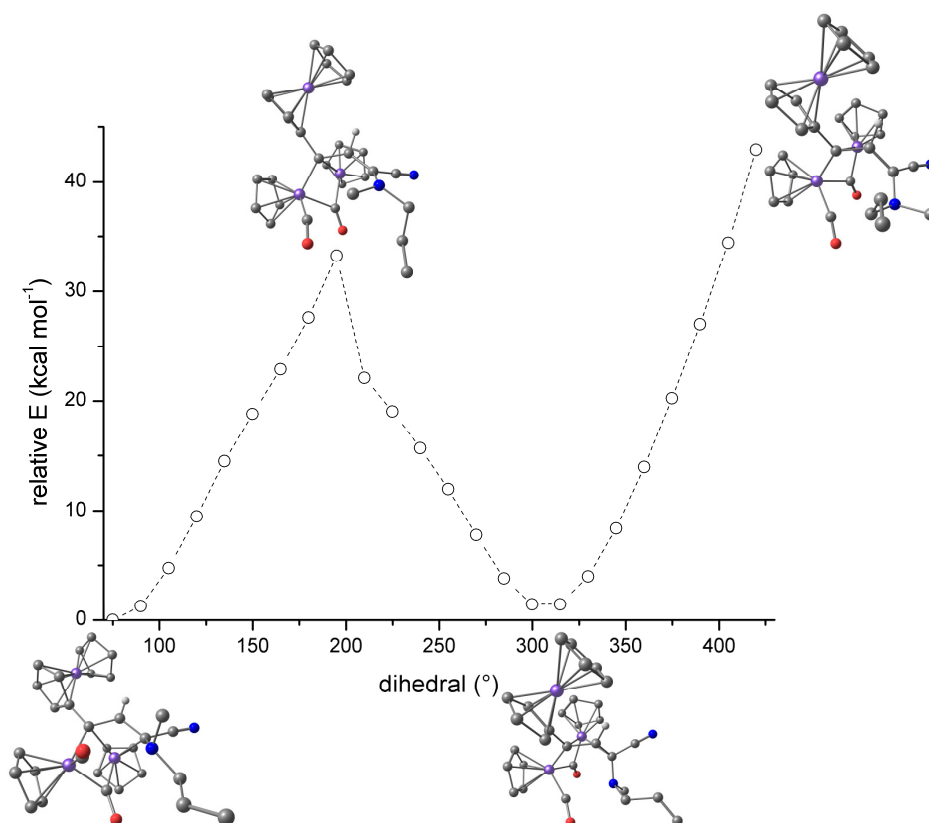


Figure S21. View of the DFT-optimized structures of the two rotamers of **2d**. Hydrogen atoms, except C²-H, have been omitted for clarity. Colour map: Fe, violet; N, blue; O, red; C, grey; H, white. Selected computed bond lengths (Å) for **(a)**: Fe1-C1, 2.044; Fe1-C2, 2.006; Fe1-C3, 2.043; Fe2-C3, 1.940; Fe1-Fe2, 2.536; Fe1-C(μ -CO), 1.921; Fe2-C(μ -CO), 1.899; Fe2-C(CO), 1.780; Fe1-C(Cp, average), 2.101; Fe2-C(Cp, average), 2.125; Fe3-C(Cp, average), 2.063; C1-N1, 1.437; C1-C(CN), 1.449; C3-C(Cp), 1.475. Selected computed bond lengths (Å) for **(b)**: Fe1-C1, 2.052; Fe1-C2, 2.006; Fe1-C3, 2.031; Fe2-C3, 1.935; Fe1-Fe2, 2.534; Fe1-C(μ -CO), 1.927; Fe2-C(μ -CO), 1.888; Fe2-C(CO), 1.775; Fe1-C(Cp, average), 2.102; Fe2-C(Cp, average), 2.123; Fe3-C(Cp, average), 2.062; C1-N1, 1.437; C1-C(CN), 1.446; C3-C(Cp), 1.474.

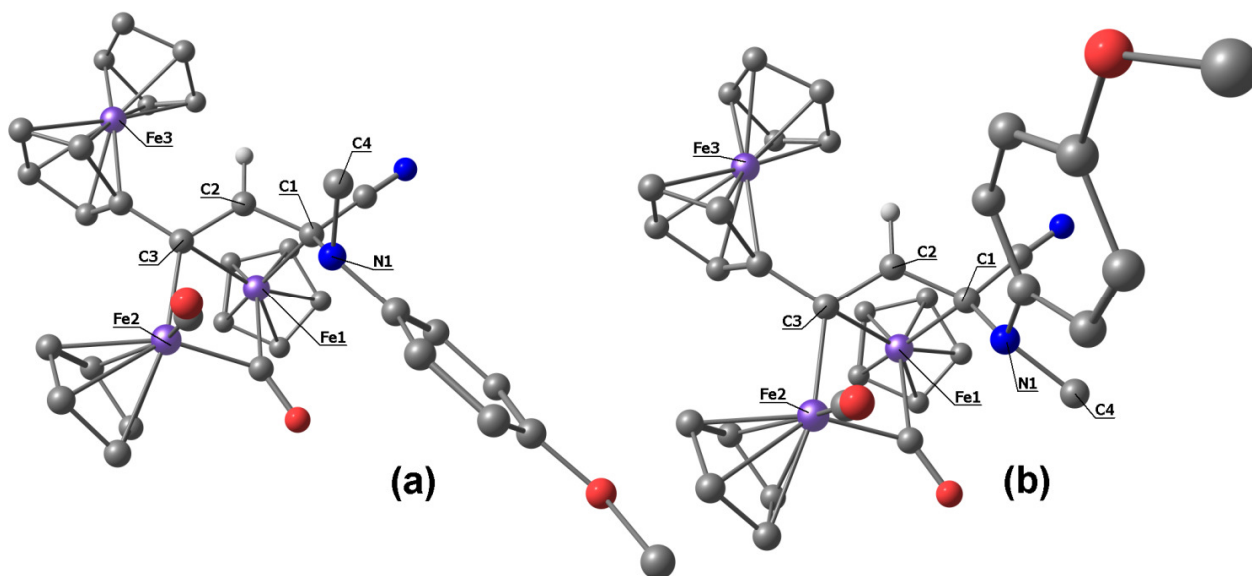


Figure S22. Relative Gibbs energy of **2c** and (**3** + ethynylferrocene).

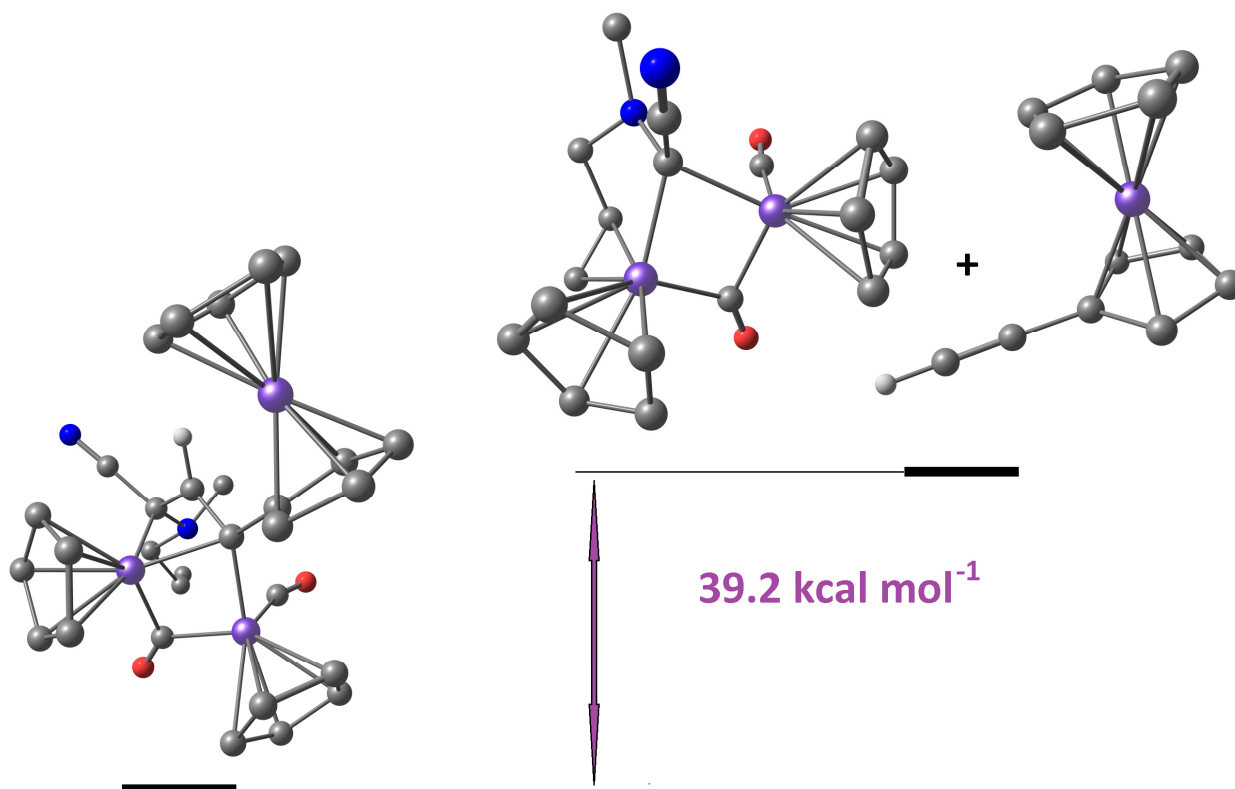


Figure S23. Relative Gibbs energy (kcal mol^{-1}) of the possible products of cyanide addition to $[\mathbf{1d}]^+$. Black text, C^1 addition, **2d** isomers; blue text, C^2 addition, **4d** isomers. Hydrogen atoms, except $\text{C}^2\text{-H}$, have been omitted for clarity. Colour map: Fe, violet; N, blue; O, red; C, grey; H, white.

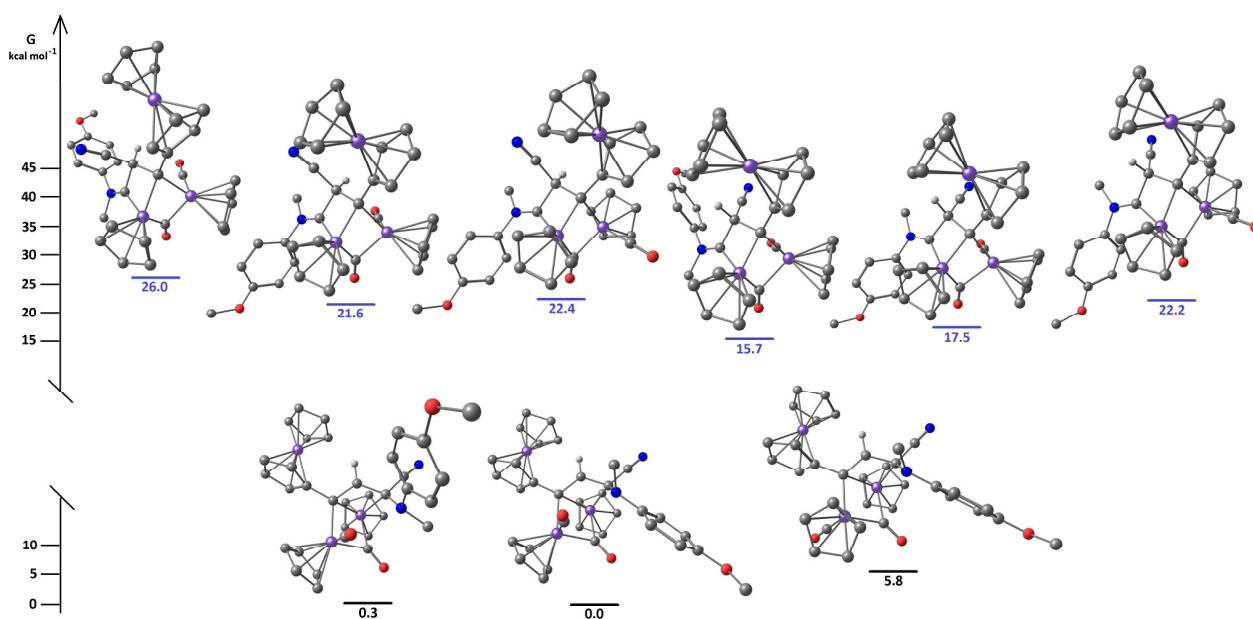


Figure S24. Relative Gibbs energy (kcal mol^{-1}) of the possible products of cyanide addition to C^1 of $[\mathbf{1e}]^+$. Hydrogen atoms, except $\text{C}^2\text{-H}$, have been omitted for clarity. Colour map: Fe, violet; N, blue; O, red; C, grey; H, white.

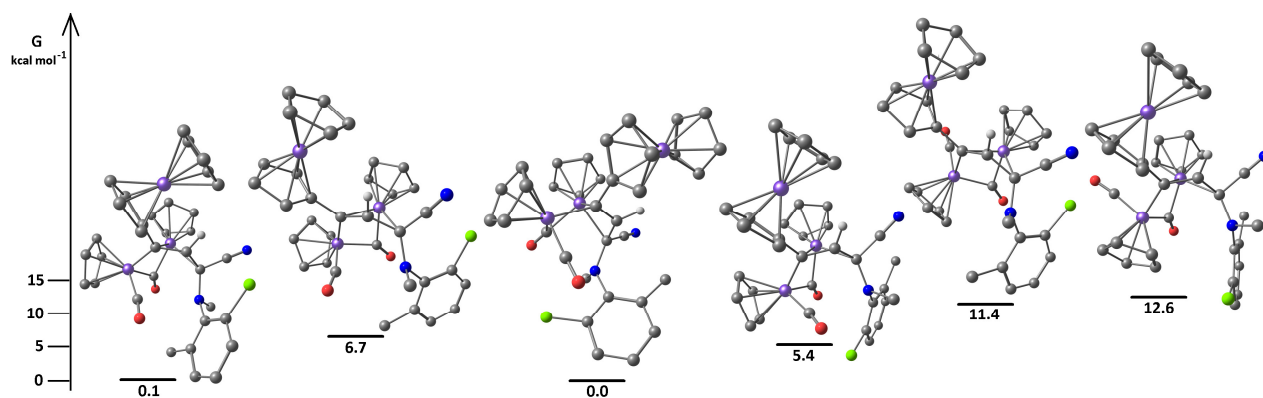


Figure S25. Relative Gibbs energy (kcal mol^{-1} , referred to the most stable isomer in Figure S20) of the possible products of cyanide addition to the C^2 of $[\mathbf{1e}]^+$, with the cyano group pointing towards $\mu\text{-CO}$. Hydrogen atoms, except $\text{C}^2\text{-H}$, have been omitted for clarity. Colour map: Fe, violet; N, blue; O, red; C, grey; H, white.

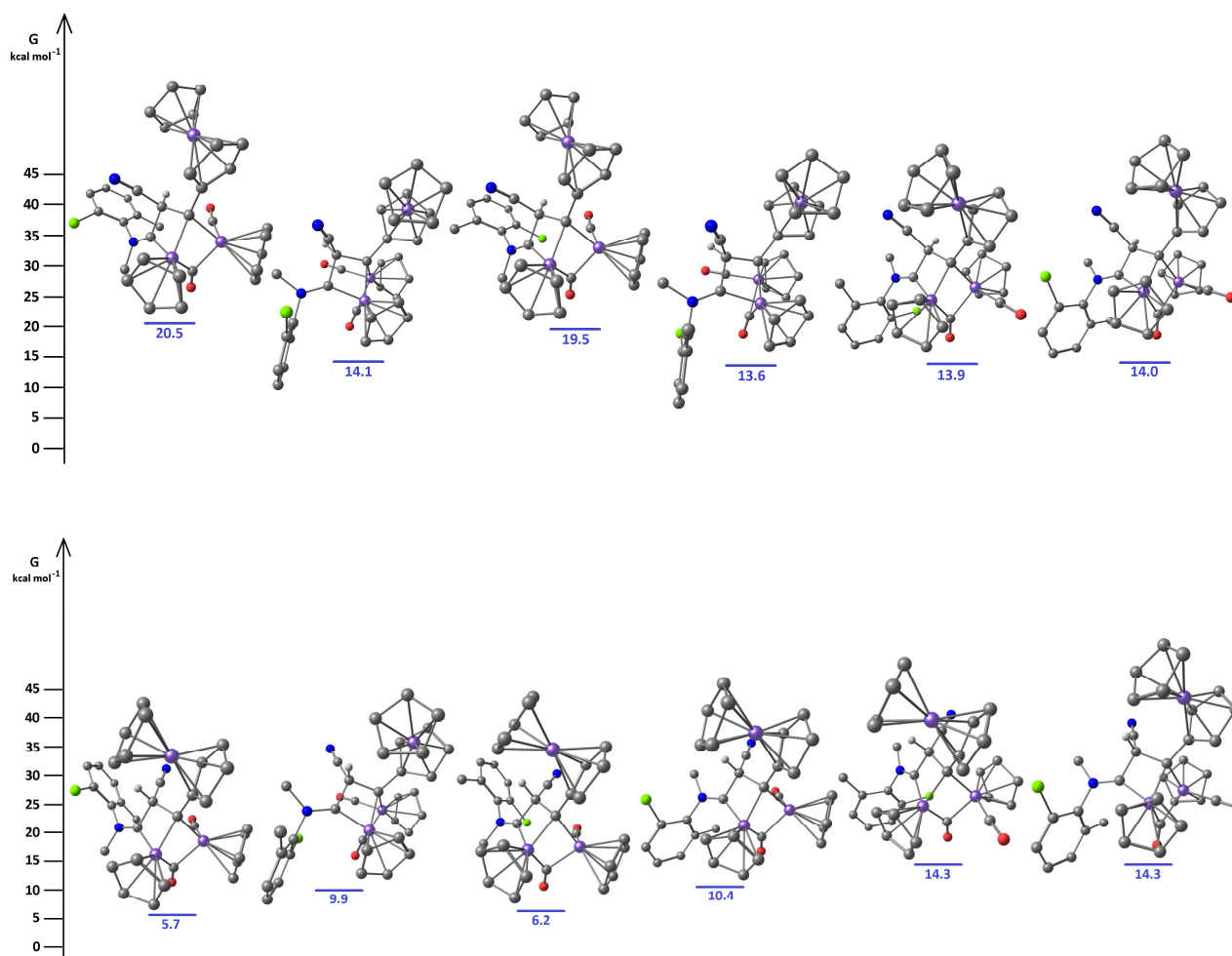


Figure S26. Computationally simulated ^1H NMR chemical shifts of the most stable isomers of **2c** and **4c**.

2c: δ 6.78 (C^2H), 6.18 ($\text{CH}=\text{CH}_2$), 5.38, 5.34 ($\text{CH}=\text{CH}_2$), 4.54 (Cp), 4.09 (Cp), 4.08 (C_5H_4), 4.02 (C_5H_4), 3.94 (Cp^{Fc}), 3.29 (N- CH_2), 1.29 (N- CH_3).

4c: δ 7.15 (C^2H), 6.45 ($\text{CH}=\text{CH}_2$), 5.78, 5.44 ($\text{CH}=\text{CH}_2$), 4.86 (Cp), 4.47 (N- CH_2), 4.03 (C_5H_4), 4.00 (Cp^{Fc}), 3.94 (C_5H_4), 3.68 (Cp), 2.89 (N- CH_3).

Simulation ^1H NMR

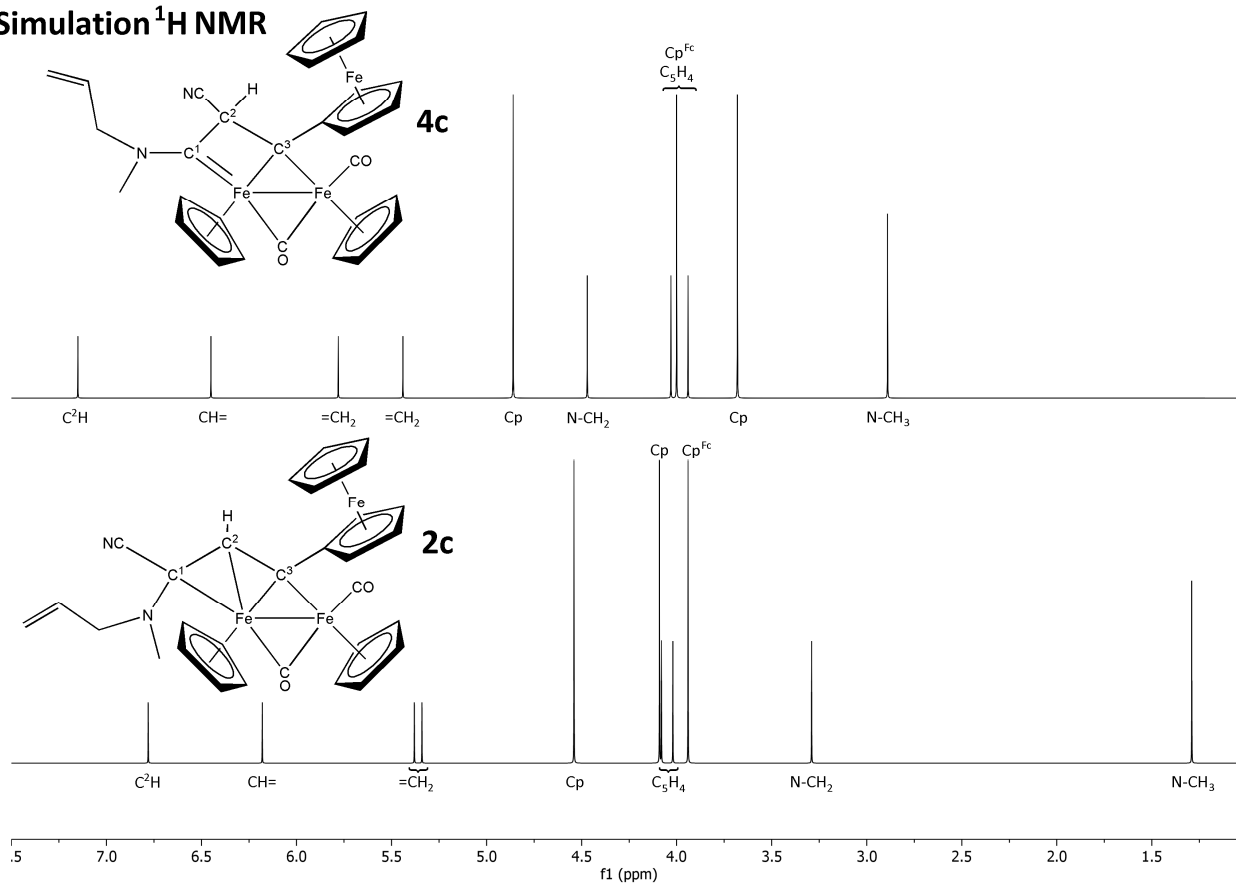


Figure S27. Computationally simulated ^{13}C NMR chemical shifts of the most stable isomers of **2c** and **4c**.

2c: δ 296.12 ($\mu\text{-CO}$), 246.36 (CO), 202.08 (C^3), 170.96 ($\text{CH}=\text{CH}_2$), 123.88 (CN), 122.27 ($\text{CH}=\text{CH}_2$), 104.48 (*ipso*- C_5H_4), 94.36 (C^2), 84.80 (Cp), 78.04 (Cp), 64.23 (C_5H_4), 63.73 (Cp^{Fc}), 61.90 (C_5H_4), 60.38 (N-CH_2), 55.16 (C^1), 46.44 (N-CH_3).

4c: δ 324.12 ($\mu\text{-CO}$), 303.01 (C^1), 254.82 (CO), 144.36 (C^3), 137.32 ($\text{CH}=\text{CH}_2$), 118.79 ($\text{CH}=\text{CH}_2$), 117.08 (CN), 110.24 (*ipso*- C_5H_4), 83.06 (Cp), 82.03 (Cp), 63.83 (Cp^{Fc}), 63.83 (N-CH_2), 63.41 (C^2), 61.56 (C_5H_4), 60.35 (C_5H_4), 44.31 (N-CH_3).

Simulation ^{13}C NMR

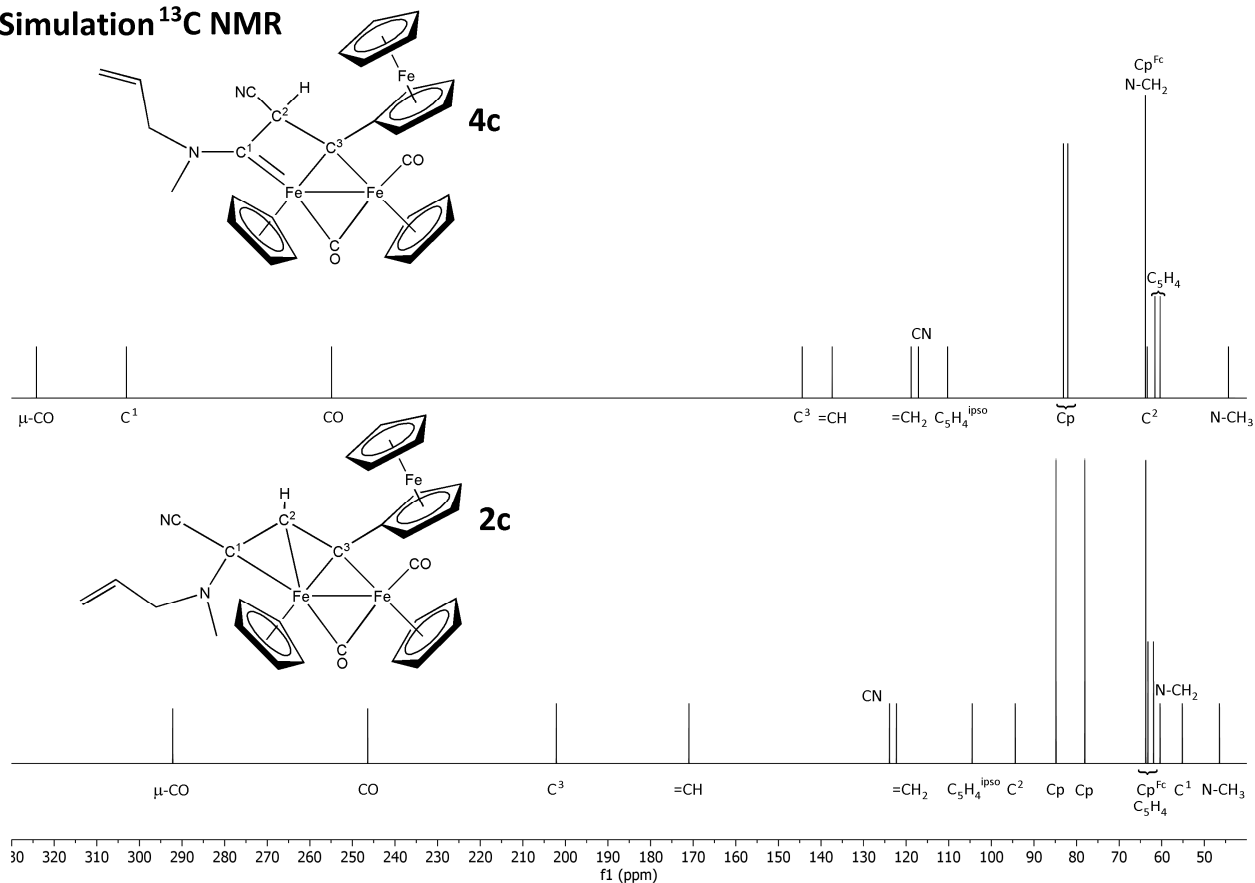


Figure S28. Computationally simulated ^1H NMR chemical shifts of the most stable isomers of **2d** and **4d**.

2d: δ 7.86 (C_6H_4), 7.19 (C_6H_4), 7.19 (C^2H), 4.57 (Cp), 4.12 (C_5H_4), 4.07 (C_5H_4), 4.04 (Cp), 4.01 (Cp^{Fc}), 3.81 ($\text{O}-\text{CH}_3$), 2.00 ($\text{N}-\text{CH}_3$).

4d: δ 7.15 (C_6H_4), 7.07 (C^2H), 7.06 (C_6H_4), 4.82 (Cp), 4.02 (C_5H_4), 3.96 (Cp^{Fc}), 3.94 ($\text{N}-\text{CH}_3$), 3.90 (C_5H_4), 3.79 ($\text{O}-\text{CH}_3$), 3.68 (Cp).

Simulation ^1H NMR

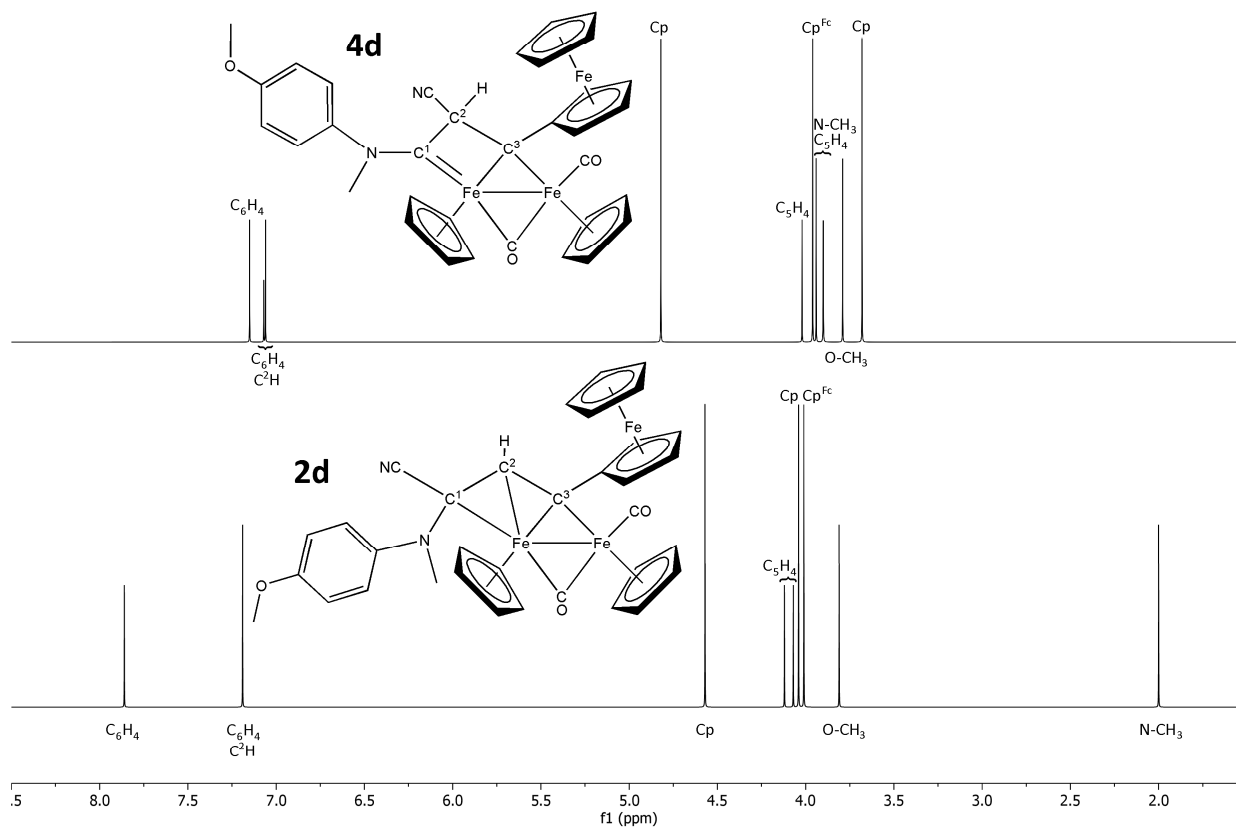


Figure S29. Computationally simulated ^{13}C NMR chemical shifts of the most stable isomers of **2d** and **4d**.

2d: δ 290.47 ($\mu\text{-CO}$), 246.78 (CO), 210.30 (C^3), 153.45 (C_6H_4), 141.75 (C_6H_4), 126.12 (CN), 124.97 (C_6H_4), 115.46 (C_6H_4), 104.06 (*ipso*- C_5H_4), 97.02 (C^2), 84.81 (Cp), 77.56 (Cp), 64.30 (C_5H_4), 63.91 (Cp^{Fc}), 61.99 (C_5H_4), 55.57 (O-CH_3), 51.20 (N-CH_3), 48.08 (C^1).

4d: δ 322.49 ($\mu\text{-CO}$), 305.93 (C^1), 254.05 (CO), 160.17 (C_6H_4), 145.25 (C^3), 136.10 (C_6H_4), 130.41 (C_6H_4), 116.78 (C_6H_4), 115.63 (CN), 110.25 (*ipso*- C_5H_4), 82.80 (Cp), 82.27 (Cp), 66.40 (C^2), 63.36 (Cp^{Fc}), 61.59 (C_5H_4), 60.27 (C_5H_4), 56.06 (O-CH_3), 51.18 (N-CH_3).

Simulation ^{13}C NMR

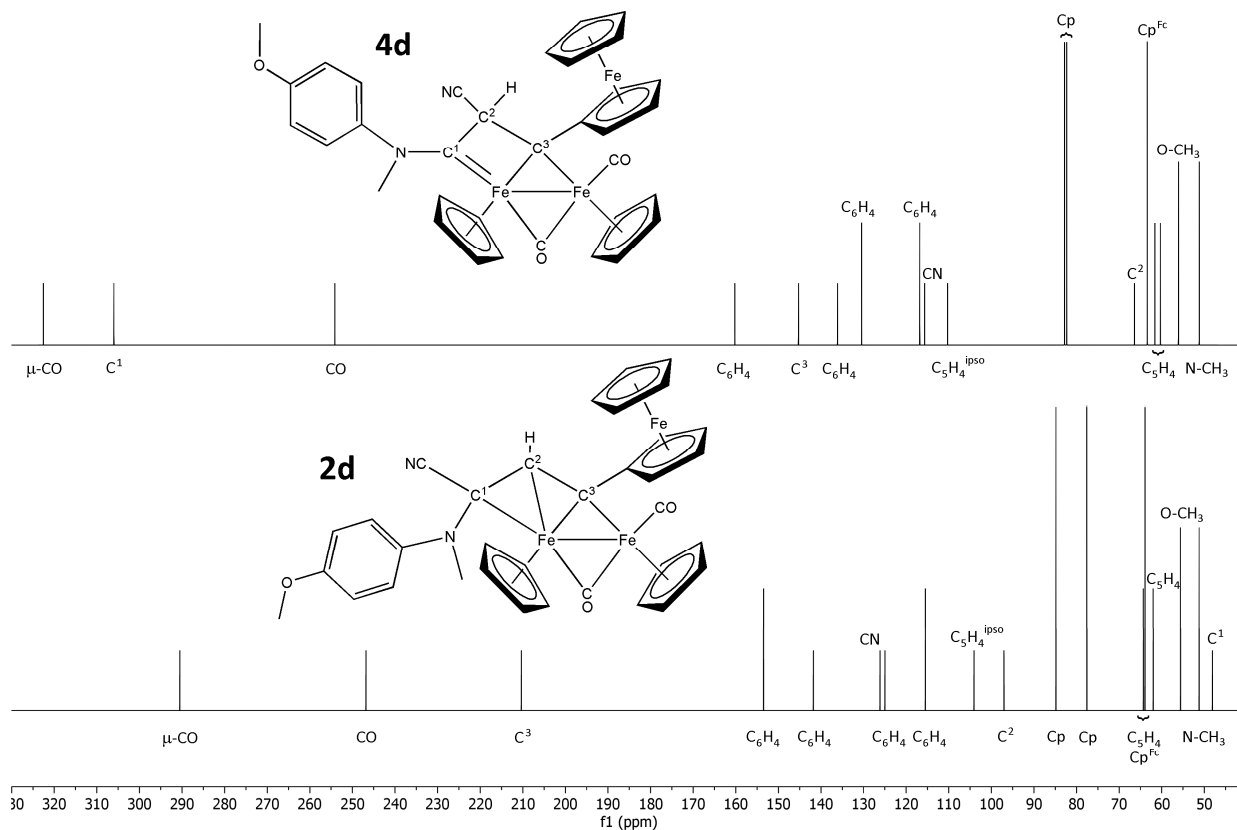


Figure S30. Hydrodynamic (blue line) and cyclic voltammetries of **2e** recorded at a Pt electrode in a CH₂Cl₂ solution between 0.0 and +0.60 V (black line), and between 0.0 and +1.0 V (red line). [NⁿBu₄]PF₆ (0.2 mol dm⁻³) as supporting electrolyte. Scan rate: 0.1 V s⁻¹.

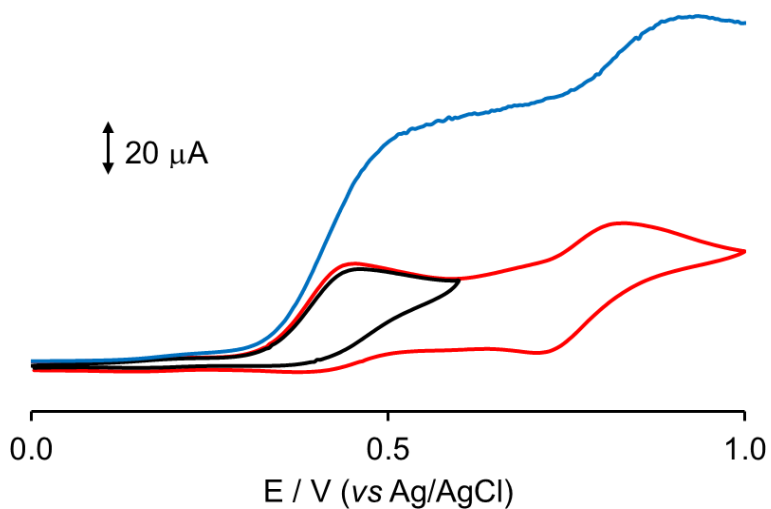


Figure S31. Hydrodynamic (blue line) and cyclic voltammetries of **4e** recorded at a Pt electrode in a CH₂Cl₂ solution between 0.0 and +0.45 V (black line), and between 0.0 and +1.0 V (red line). [NⁿBu₄]PF₆ (0.2 mol dm⁻³) as supporting electrolyte. Scan rate: 0.1 V s⁻¹.

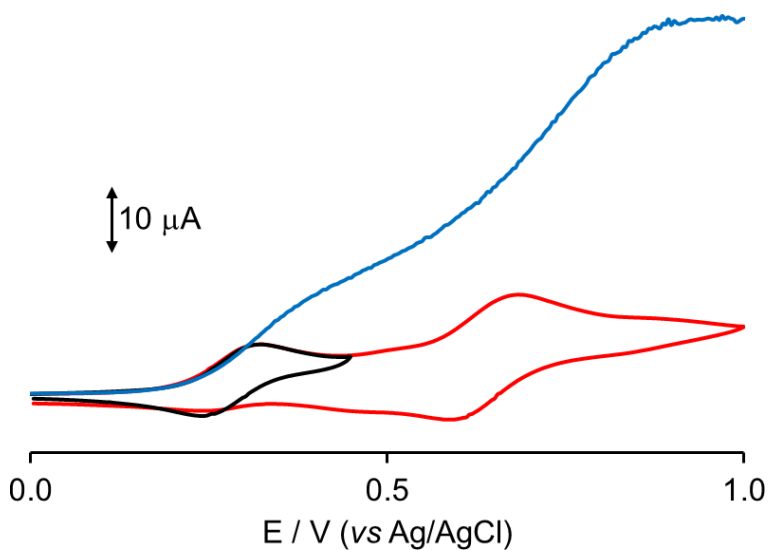


Figure S32. Hydrodynamic (blue line) and cyclic voltammetries of **5b** recorded at a Pt electrode in a CH₂Cl₂ solution between -0.2 and +0.3 V (black line), between -0.2 and +0.56 V (red line) and between -0.2 and +1.0 V (green line). [NⁿBu₄][PF₆] (0.2 mol dm⁻³) as supporting electrolyte. Scan rate: 0.1 V s⁻¹.

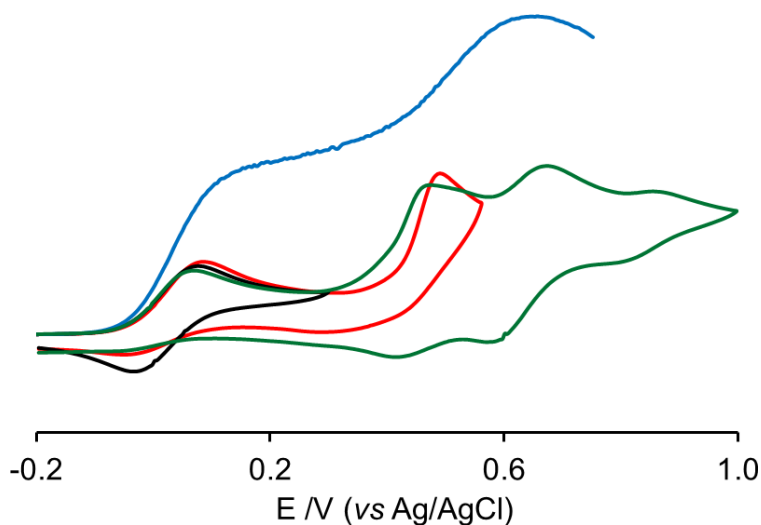


Figure S33. IR spectra of a CH₂Cl₂ solution of **5b** recorded in an OTTLE cell a) during the microelectrolysis at the constant potential of +0.35 vs Ag pseudo-reference electrode and b) before (black line) and after (red line) two consecutive microelectrolysis cycles at the potential of +0.35 and -0.3 V (vs Ag pseudo reference electrode), respectively. Starred peaks are due to decomposition products. [NⁿBu₄][PF₆] (0.2 mol dm⁻³) as the supporting electrolyte. The absorptions of the solvent and supporting electrolyte have been subtracted.

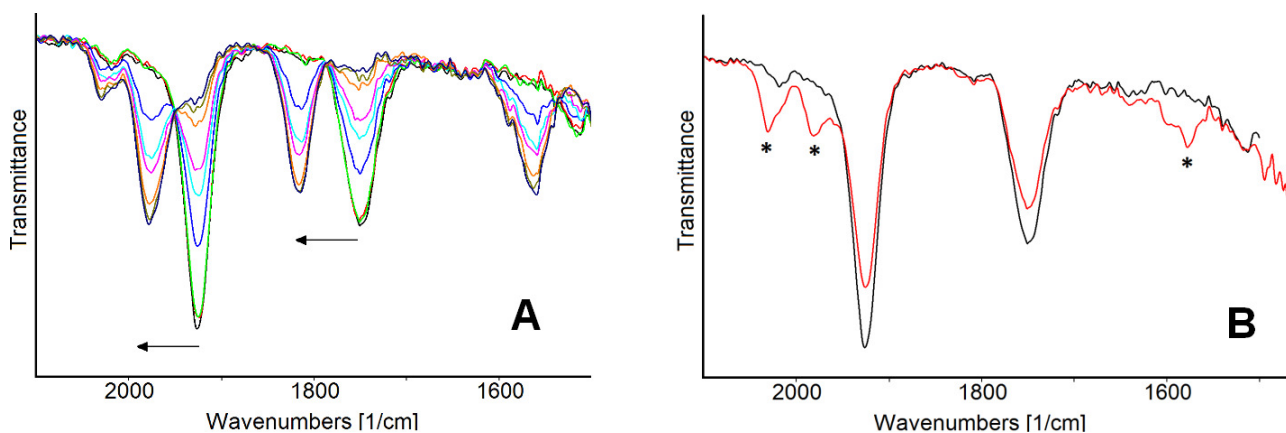
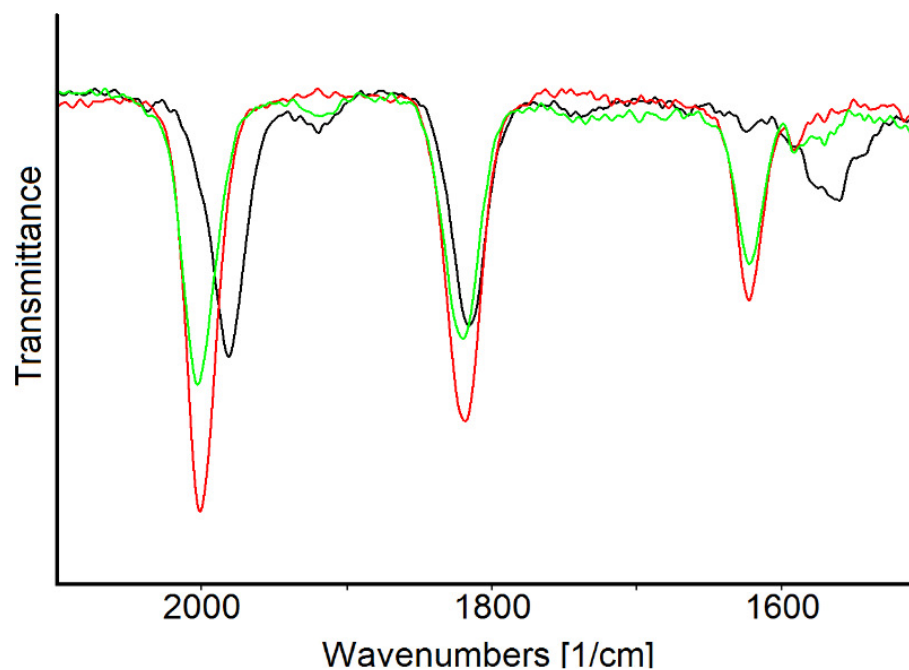


Figure S34. IR spectra recorded in an OTTE cell of a CH_2Cl_2 solution of **[6]⁺** (black line), **[1e]⁺** (red line) and of the product (green line) obtained at the end of the microelectrolysis of **6** at the constant potential of +0.90 V (vs Ag pseudo-reference electrode) $[\text{N}^n\text{Bu}_4][\text{PF}_6]$ (0.2 mol dm^{-3}) as the supporting electrolyte. The absorptions of the solvent and supporting electrolyte have been subtracted.



Cartesian coordinates of the DFT-optimized structures

65

[1c]⁺ + CN⁻ (C1-CN, is1)

Fe	1.94694749124146	1.35546046046827	0.23874980514800
Fe	1.44326071688591	-0.99937283569554	-0.52883556414585
C	0.21185319649395	-0.36105211391384	-2.03874615436187
C	3.09952401576546	-2.29212657263656	-0.45894024031075
C	2.09447682191625	-2.82525433396006	-1.29411190174317
H	3.10648766780171	-1.80758817503006	1.71792792621948
H	2.18857909576942	-3.03663451153051	-2.34912486799268
C	0.93553731063351	-3.01585240073682	-0.50053413308396
H	-0.00897109763240	-3.41682022711152	-0.83796557092516
C	1.23847993902647	-2.61738693002542	0.82380920682318
C	2.56955922677510	-2.16443548437838	0.85301437159462
H	4.10888346309735	-2.04906900319439	-0.75665528508811
C	2.67468032982161	0.29665412647692	-1.17689700194369
O	3.55274904785093	0.39014260217919	-1.93335104843685
H	4.39220751443002	2.84094264318629	0.02682581228457
C	3.70330825102438	2.41846160282305	0.74319260966882
C	3.76613638402923	1.12674883417987	1.30812097413815
H	2.25128748834773	4.08009221019500	1.09535837731725
H	4.51274983686574	0.37626999754435	1.08840979327882
C	2.68537028370812	0.97746314883924	2.20858847271297
H	2.47779583266884	0.10789218254426	2.81020026436383
C	1.94789155072584	2.18237562888199	2.20895585849846
H	1.05905663421695	2.39037512029163	2.78537356408607
C	2.56928867123550	3.06834171597510	1.30465099811318
C	-1.82657546700257	0.91585158267202	-3.91457167118651
H	-2.38840786528821	0.12421260504232	-3.42777545646246
C	-2.13198828495623	1.24408201865078	-5.16437054543419
H	-2.91947766101381	0.74056392012660	-5.71008250678338
H	-1.60601500926811	2.03437948988628	-5.68807795690798
C	-0.75481165206838	1.59397302391060	-3.10859580710309
H	-1.17545553754598	1.89996469778410	-2.14765509817675
H	-0.44010944327123	2.50378979966400	-3.62558709207527
N	0.45204807006269	0.80182111156145	-2.84483049230984
C	1.20780365250334	0.55363856758451	-4.05850060503807
H	1.58670935216667	1.49890768412925	-4.44921937903715
H	0.61680344042225	0.07830214093481	-4.85081395741376
H	2.05729078020978	-0.09146593003284	-3.85234814366118
C	-0.28188790458008	-1.48687651224539	-2.79948169215066
N	-0.62223257141314	-2.38037709493609	-3.44897225394966
H	0.55215401549936	-2.64161608439526	1.65756894267609
C	1.34541370882295	2.50880489856401	-0.97489845601949
O	1.07922457200551	3.43679268078319	-1.57977811712353
C	0.24392963629339	0.42587819962534	0.31797843278812
C	-0.39815301187552	-0.21938859750405	-0.73609259904472
C	-0.50982550576768	0.51315209146876	1.58425948062989
C	-0.27515896998405	-0.09478718188304	2.84647350397076
H	-1.98011298950478	2.07722134141678	0.98893076549629
H	0.45795327564226	-0.85934589717485	3.05578114344788
C	-1.15812975157060	0.47817220863342	3.79813561117928
H	-1.22099683876826	0.21174415516065	4.84376973727465
C	-1.95843338388503	1.43592643401816	3.12852091917867
H	-2.73940262470042	2.03740878373681	3.57163912843720
C	-1.57005773767120	1.44559452003346	1.76520783743771
Fe	-2.23659169502459	-0.42118699304661	2.30752573409794
H	-5.02046599391282	0.03513511177737	2.15463239840882
C	-4.26366245473380	-0.73507033575011	2.11111856373383
C	-3.75719029497202	-1.46896794303141	3.21387318037734
H	-3.75971452957332	-0.81520848584485	-0.06029234647738
H	-4.05848703779206	-1.35411509531399	4.24539196499138
C	-2.77404280980434	-2.36706553549229	2.72836999463368
H	-2.19646176607245	-3.05982494852228	3.32344052774584
C	-2.67438802726270	-2.19035761226278	1.32522600891179
H	-2.01785476933040	-2.73739894299106	0.66329062676398
C	-3.59521474672901	-1.18135897505912	0.94330464026789
H	-1.28877184098452	-0.80198558705072	-0.51672923230927

[1c]⁺ + CN⁻ (C1-CN, is2)

Fe	1.47904371666366	1.47283450837981	0.33462163358026
Fe	1.25574984278536	-0.86558400136652	-0.61217458062297
C	-0.08085663960509	-0.25588122887514	-2.03183214857897
C	3.04206450110508	-1.96852889883983	-0.68615151230471
C	2.07152241940844	-2.54789414274554	-1.53147760622248
H	3.06815997825812	-1.63303015188038	1.51912581258757
H	2.15084037411292	-2.67511934170864	-2.60138842301752
C	0.96584949205431	-2.91614294704201	-0.72398926733830
H	0.05925419803568	-3.39113988137823	-1.07001830060779
C	1.26735090247983	-2.57814509086859	0.61816974490619
C	2.54472146882248	-1.98832729569040	0.64516309609658
H	4.00873089057497	-1.59622469077632	-0.99202944789293
C	2.32018732320746	0.62237985789481	-1.14601474322396
O	3.17689678118430	0.87851431172764	-1.88991364835275
H	3.59596749415175	3.39537556990033	0.13053971430567
C	3.03936070536943	2.80235446681607	0.84128188141224
C	3.37045716638518	1.50974918827816	1.29960298615955
H	1.33343296244265	4.13753459979633	1.39428188812375
H	4.22636828227652	0.92795506549925	0.98740769251348
C	2.38932352764805	1.09858779529941	2.23373543336831
H	2.38858979868772	0.17017125368068	2.78172673298239
C	1.44794839511308	2.14336842770403	2.36376921557604
H	0.57062743994069	2.13863161222352	2.99288482229778
C	1.84173859715029	3.18995329451759	1.50509750579186
C	1.34453902234644	2.24089245462643	-4.37989311769525
H	1.95760176782871	2.76014641369273	-3.64980586893590
C	1.11706010864217	2.80120188331426	-5.56128320994312
H	1.53421751972831	3.76489778855555	-5.82264730420309
H	0.50657305637709	2.31495680153067	-6.31346090940520
C	0.82389773871691	0.89874220774328	-3.97050625026452
H	1.66357081552218	0.22650261332988	-3.78802763163555
H	0.25166703218422	0.45819263564749	-4.80116270870903
N	0.01789253000756	0.98264338680443	-2.75580792112527
C	-1.29555576758400	1.53786518729944	-3.05026615968037
H	-1.19335564582257	2.52098131822738	-3.50850455753701
H	-1.87154829944104	1.65036059182604	-2.13328751583176
H	-1.87120167167011	0.90582738982968	-3.74077824880757
C	-0.53168792178867	-1.33766394414737	-2.88074303607076
N	-0.86204446196251	-2.16944881488926	-3.61146355509946
H	0.60593154224255	-2.71374469189666	1.46047706198891
C	0.59550154637151	2.57669275793680	-0.74735110140626
O	0.07666482141340	3.47661849499646	-1.21496653454324
C	-0.07356739556606	0.31530452090255	0.39150194029620
C	-0.66927166473514	-0.29364798797559	-0.70976595505670
C	-0.78279629816384	0.18450248506474	1.67959985543661
C	-0.38145909123668	-0.44926689259693	2.88573484677540
H	-2.54221130808180	1.48239956704816	1.24864827671424
H	0.49072089678255	-1.07223440648914	3.01361286700284
C	-1.30890974973005	-0.11463828331913	3.90475405213773
H	-1.27264667200351	-0.45443072648465	4.93022695701901
C	-2.30339052659667	0.71695382191677	3.33380950043873
H	-3.15946371155416	1.13216767722413	3.84635963954493
C	-1.98635344940866	0.89039498375006	1.96277437479058
Fe	-2.27073395898356	-1.10266679526504	2.38550076056534
H	-5.09433252609342	-1.18297047904887	2.37278909855366
C	-4.20800034239255	-1.78434785373490	2.22985263935865
C	-3.51562978724131	-2.50184193229091	3.23832758012773
H	-3.80607150777616	-1.56843711701311	0.04636279069170
H	-3.77993623806521	-2.54131304671683	4.28550237823772
C	-2.40705721747063	-3.14758493090624	2.63503879091960
H	-1.67977765030532	-3.76749513861054	3.13974852653871
C	-2.41725820914328	-2.83163944935109	1.25387154834243
H	-1.70393354380920	-3.17583705727744	0.51972782871614
C	-3.52766465397458	-1.98631145196617	1.00335779046919
H	-1.47692274581582	-0.99957026183309	-0.53649400025532

[1c]⁺ + CN⁻ (C1-CN, is3)

Fe	1.10385916771147	1.66380664559441	0.18397990456331
Fe	1.18123943949564	-0.74271359997510	-0.75648977455933
C	-0.14140589646766	-0.26255421311349	-2.21894164149469
C	3.05279054918515	-1.70248437372335	-0.99127014312668
C	2.05683660092030	-2.38371647679968	-1.71585791449515
H	3.28595146251755	-1.32385675498122	1.19277213969939
H	2.03851079783927	-2.53521499967447	-2.78520740880353
C	1.07013846204995	-2.81407119928957	-0.79476285446379
H	0.18049088722693	-3.37280197518412	-1.04436899961899
C	1.47684004357445	-2.41812483321424	0.50510817369528
C	2.69704229881838	-1.72935589144474	0.38556885257847
H	3.95108393579222	-1.26840293231216	-1.40356263739792
C	2.17113499829819	0.90029082316688	-1.18996909695236
O	3.02451043129409	1.20476950679247	-1.91043607487597
C	1.34193994246106	2.05616034982744	-4.71367928193562
H	1.91314354279707	2.67244067411714	-4.02622204571840
C	1.15981092613690	2.46866394391070	-5.96215840264245
H	1.57011913988583	3.40497479543352	-6.31699275726283
H	0.59618431695658	1.88124674691466	-6.67790789500989
C	0.83780953245765	0.75368577292989	-4.17504224012717
H	1.69109833407521	0.13833448815537	-3.88143969776545
H	0.32128388890702	0.20501113814363	-4.97878911448212
N	-0.01416892313165	0.93371946165584	-3.00548077145333
C	-1.30543325715253	1.48916839723386	-3.37078787315360
H	-1.17293540911819	2.44797338936808	-3.87281084894374
H	-1.90230344713808	1.66182857965598	-2.47679237038986
H	-1.87948015397591	0.83512937061145	-4.04388133706381
C	-0.53749164699210	-1.39660750784550	-3.03263733906660
N	-0.82646762883271	-2.27752974320976	-3.72243589406355
H	0.93448990716844	-2.60197766440811	1.42109050555075
C	-0.26667805676386	0.29227281565477	0.21631579979780
C	-0.79042902237224	-0.30724670511519	-0.92127402947275
C	-1.00941822093094	0.12813633480490	1.47801648877414
C	-0.57713051669768	-0.37051066306555	2.73782784141285
H	-2.91188655164850	1.13930875613170	0.90492134734964
H	0.35871429916428	-0.86902581561167	2.94285260765452
C	-1.58852565129649	-0.11249276739633	3.69775340608563
H	-1.55218178441153	-0.38536429042512	4.7429288006880
C	-2.66114592919874	0.53870543987712	3.04116864137284
H	-3.58761128842419	0.85953339175123	3.49574102432940
C	-2.31180800414300	0.67354316649021	1.67456578147878
Fe	-2.33742351854290	-1.30714238886998	2.20883104602935
H	-5.11236915424860	-1.81864394078287	2.35924170829160
C	-4.15384487698933	-2.27777898045480	2.16393321832306
C	-3.30359981052268	-2.87413007328588	3.13015980809310
H	-3.91191866935320	-2.01683679011605	-0.03950991565595
H	-3.50092581695457	-2.94767635638032	4.19015552235075
C	-2.14316683000284	-3.34299513587272	2.46391496481485
H	-1.30138589470796	-3.83951999831198	2.92507247461745
C	-2.27956696788261	-3.04039661538596	1.08565302527852
H	-1.56413265854788	-3.26943760418835	0.31093277325705
C	-3.52029545989570	-2.38039228413678	0.89988178139648
H	-1.57013501972499	-1.05425474804718	-0.78162114471306
C	1.98764462505499	1.06525123517257	1.59173054405036
O	2.56919766908954	0.80450214827309	2.53609433900068
H	2.77677875260198	3.86831272994222	-0.69508397932930
C	1.79153395531037	3.62431000899345	-0.32631170793811
C	1.39857660796785	3.59454464036272	1.02439930880191
H	0.61303932530287	3.27713052154767	-2.19143179614307
H	2.03849208852413	3.79448007505395	1.87283939084747
C	0.03054390600429	3.22275764028212	1.08716844818397
H	-0.56091315823922	3.11566643772037	1.98446740814918
C	-0.43008273526740	3.07784587743681	-0.24832139567234
H	-1.43584985841606	2.81825336428488	-0.54111480829568
C	0.64725198340228	3.32046165531116	-1.11622316381023

[1c]⁺ + CN⁻ (C2-CN, is1)

Fe	1.82992432953833	1.27306491291344	0.20739929991709
Fe	1.58658210828119	-0.90984760017299	-0.89530151484027
C	0.14801161883433	-0.36111117597032	-1.97569443505694
C	3.42456780763983	-1.97132772846337	-0.55629256146678
C	2.92890514948180	-2.26272448990450	-1.85436135566739
H	2.53636949073520	-2.27300699526635	1.46210440076176
H	3.44379749316233	-2.08323186545001	-2.78674752225230
C	1.65674097475527	-2.85463965420708	-1.69993565006661
H	1.01442570698068	-3.19906216681157	-2.49837099652255
C	1.35802131505044	-2.91748261693888	-0.31797943400616
C	2.46086730287465	-2.37139334049925	0.38910239338230
H	4.37708879854186	-1.50922174874868	-0.34056707354564
C	2.38346010108286	0.60793227762850	-1.51909677714836
O	2.99242041035394	1.04931223091395	-2.42234419009999
H	3.15723357951277	3.78952655127661	0.28681361535030
C	3.09809391591108	2.84064395031710	0.80070541531597
C	3.89178356327151	1.71055242736638	0.54727950571297
H	1.48925567674596	3.18798517251209	2.31739660988355
H	4.66537860623447	1.63191353433248	-0.20215004406410
C	3.50672854989969	0.68935523051010	1.45834499369221
H	3.95945466432931	-0.28456616840127	1.54354337469374
C	2.48690773616817	1.19363402883635	2.27896252958409
H	1.98856142645823	0.65146193161778	3.06650286723803
C	2.20016371413164	2.51295495454377	1.86307113694653
N	-0.20171295668400	-0.27212571909594	-3.21908453375120
C	0.68809961934637	-0.69852566541659	-4.29164925166547
H	0.71383171424416	0.05831195333200	-5.07357070209093
H	0.31982057199797	-1.63094868349872	-4.72008325273599
H	1.69018817294648	-0.84999027062314	-3.91038707403531
C	-1.60923030347202	-1.22405263410731	-0.76057297986075
N	-2.19837438989247	-2.21195520242004	-0.82222268472912
H	0.46508117176057	-3.34352565273376	0.11226246591631
C	0.67798782779303	2.37578494079907	-0.48467336696508
O	-0.07940654674079	3.16092998675494	-0.83347114275442
C	0.29563335138486	-0.00989352369413	0.27634661642252
C	-0.77944121297031	-0.01999283886345	-0.83338110351316
C	-0.24162709678420	-0.23985600979328	1.64879882232821
C	-0.50252156516301	-1.47210077925714	2.30953827599359
H	-0.39467853707051	1.84368284520652	2.43194819800766
H	-0.43706809636313	-2.45200540550334	1.86208133728954
C	-0.82139867075863	-1.21523761958359	3.66900520799570
H	-1.04116774395604	-1.96048629625499	4.42069149963132
C	-0.79712308956840	0.18754763239034	3.86142589214055
H	-1.00770666507092	0.71137472717475	4.78334687158641
C	-0.48700273101985	0.78321556522072	2.61305068275223
Fe	-2.21551692497889	-0.28864538396021	2.48886450151341
H	-3.63187302006885	2.12292389169315	2.04760006930707
C	-3.74914158402773	1.05542707442818	2.16904789652717
C	-3.93811275443428	0.37159235622159	3.39578553472683
H	-3.64788442054087	0.30756348134852	0.07528310835724
H	-3.97840459647934	0.82557870901960	4.37577906311302
C	-4.04253553367643	-1.01440536785955	3.11382569531554
H	-4.18332370143688	-1.80115008126642	3.84132178502940
C	-3.91605946840353	-1.18806803816074	1.71424875909303
H	-3.94725800491412	-2.12781090704550	1.18453122666221
C	-3.73992344701811	0.09252587441278	1.12940412590265
H	-1.45129227309044	0.84739650470472	-0.93419559184522
C	-1.49988136770955	0.21447886225803	-3.68049487047180
H	-2.24702158331112	0.09460434374841	-2.89563774199123
H	-1.82668688419792	-0.43435385973016	-4.49738647019431
C	-1.48258198286004	1.63858068777259	-4.14305896596426
H	-2.42237021271280	1.96909833983288	-4.57275626605419
C	-0.46384120328033	2.48266515688337	-4.06326837690406
H	-0.56074715082573	3.49877167644782	-4.42001856789734
H	0.49835625003229	2.20849567728376	-3.64929527992921

[1c]⁺ + CN⁻ (C2-CN, is2)

Fe	2.01827611041502	1.28387469278624	0.13054037247307
Fe	1.32451416621542	-0.92694623252843	-0.77179240445999
C	0.23785564520064	-0.05182273474353	-2.05237688386666
C	2.73442374087630	-2.53481258683429	-0.57218440796392
C	1.81188196569004	-2.80694532815751	-1.60508860223944
H	2.45584888862619	-2.19130081884090	1.60827285009102
H	2.05106493594537	-2.99367539191561	-2.64146043883612
C	0.51344212963927	-2.82806704695324	-1.02610451614417
H	-0.41192448178354	-3.02795113069548	-1.54688549374137
C	0.64831656166746	-2.58039925105784	0.35911959437908
C	2.02121040690606	-2.39092729526407	0.64107616313359
H	3.80549070726840	-2.44470273771029	-0.68758770970099
C	2.66715055739487	0.14659677882340	-1.32093119432463
O	3.56676027024227	0.24670722294751	-2.07105059040967
H	4.46310039284506	2.75620921185234	-0.09240419861717
C	3.80369233981238	2.29040065665442	0.62534569430905
C	3.88792528193143	0.96698381795694	1.10309481070551
H	2.37517857231142	3.93221259508617	1.14957079770179
H	4.61857267257484	0.22984482475294	0.80168266775203
C	2.84792899311536	0.76212601380356	2.04005424682158
H	2.66938589860026	-0.14512178435659	2.59168953618739
C	2.11362244986920	1.96426368118496	2.14978463778994
H	1.25343574288389	2.13449715971859	2.77944922103448
C	2.69467073003370	2.90699435616729	1.27615589528961
N	0.08965433379789	0.07126728821352	-3.33319198899690
C	-0.88694024711061	0.93426703551732	-3.99225390604523
H	-1.59164210403160	0.33162669074816	-4.56221896222096
H	-0.36506493156115	1.60267364044134	-4.67568913009995
H	-1.43658166415204	1.53561318031038	-3.27724561200673
C	-1.93798184553670	-0.01151853174713	-1.14553670122451
N	-2.93525392327251	-0.54584753013020	-1.36019520598432
H	-0.16038119130767	-2.52198350167937	1.06985872496890
C	1.50722169751527	2.43633200924348	-1.07602919023971
O	1.23886168161583	3.26240567233169	-1.82200993427436
C	0.23739578304338	0.37236276629798	0.15831772876276
C	-0.65112318476010	0.67594349767061	-1.06062298481261
C	-0.44273578506031	0.39357051689804	1.46413378904116
C	-0.06554920726323	-0.26137209747310	2.67048714706040
H	-1.99656486446466	1.96617817920701	1.13341655764991
H	0.68242048297220	-1.03418675317812	2.76129304416178
C	-0.78120026764441	0.30712005374164	3.75506016716134
H	-0.68831260312294	0.02755250793418	4.79534114467500
C	-1.66625614813119	1.27855386887424	3.22529151428021
H	-2.36703985168789	1.87983363074422	3.78743958633603
C	-1.48077247352557	1.30694933100874	1.81890975840174
Fe	-2.08360914817251	-0.57092842250336	2.46107183621232
H	-4.67601780817124	-0.24363089595487	3.52490257824097
C	-4.02731211116171	-0.94935866116982	3.02579495373986
C	-3.14456634692172	-1.86160865806312	3.65942018022794
H	-4.42690540023991	-0.55693365726755	0.86797767418003
H	-3.00448113180233	-1.97373981295264	4.72518824610542
C	-2.47127107706989	-2.59207306082923	2.64826135278385
H	-1.73076013775711	-3.36309059202782	2.80959280509652
C	-2.93478905605782	-2.13058959526612	1.39125579895794
H	-2.61642679870006	-2.49311207807825	0.42576982723658
C	-3.89419808055697	-1.11193497369551	1.62482762295493
H	-0.87941652076202	1.73344416698581	-1.26007011332817
C	0.90956914627171	-0.70607129663475	-4.25502674547808
H	1.83900966937566	-0.97631992367870	-3.75698982223197
H	1.18525768843339	-0.05964061015672	-5.09222625450393
C	0.23731273281225	-1.93861437693572	-4.77614415220856
H	0.79342016086269	-2.43714406821164	-5.56347752134453
C	-0.91436430571392	-2.45213779438093	-4.36541974061810
H	-1.30145197329156	-3.35969894036980	-4.80793965812077
H	-1.51679886597022	-2.00397587646032	-3.58455846186016

[1c]⁺ + CN⁻ (C2-CN, is3)

Fe	1.57774873598429	1.59466281237853	0.06700475102047
Fe	1.38906617897738	-0.92340689668272	-0.93979133205959
C	0.24600951930405	-0.07492891105562	-2.19496128133716
C	2.72413312180201	-2.57888995224887	-0.69355268966309
C	1.81607853118046	-2.81522470916807	-1.75337770112261
H	2.40605445310144	-2.19012515493305	1.47384849487626
H	2.07538277375700	-3.01867959796659	-2.78167111167507
C	0.50615115716259	-2.80451729762094	-1.20176280998288
H	-0.41277438131758	-2.98381887381010	-1.74070099271184
C	0.61635880553672	-2.53917355246268	0.17914026104881
C	1.98981793801209	-2.38775506706327	0.49742647451189
H	3.80066026374842	-2.53609129315739	-0.78389589424499
C	2.80446176644179	0.00442991825562	-1.37700745182024
O	3.82333449856893	0.33246723795515	-1.80765771155433
N	0.11019253011866	0.06453287632833	-3.47543505588673
C	-0.96589333409337	0.81534216110198	-4.12121064684719
H	-1.75262888956154	0.14700826988028	-4.46625879956682
H	-0.55912979874358	1.34539497973602	-4.97948923208829
H	-1.39482881838286	1.54650049902225	-3.44369979445983
C	-1.96401465186079	-0.24523491949798	-1.33923097034658
N	-2.92559510189549	-0.84119024971906	-1.55513994158372
H	-0.20271893334684	-2.45307796692161	0.87201128381462
C	0.12337287796567	0.35151163177444	0.05248200292302
C	-0.73672455929239	0.53601354209811	-1.21750149264869
C	-0.61707905892742	0.23616955321601	1.32483505841132
C	-0.18727467213711	-0.34896764109259	2.55021368226416
H	-2.36104412543388	1.58254522930019	0.93521198065825
H	0.65605475535612	-1.01356041513443	2.66680738019326
C	-1.00599537229122	0.12600219487963	3.60808585898691
H	-0.90375909711241	-0.12862281296438	4.65377546915791
C	-1.99737890158513	0.96325486811453	3.04264147350845
H	-2.78792759979114	1.47052586372756	3.57795184866370
C	-1.78018826950321	1.00268677932467	1.64027107734052
Fe	-2.14923041922950	-0.92681344954406	2.28984045349271
H	-4.74483797113392	-0.94611574627446	3.39587488719157
C	-4.02596758512959	-1.55178378533542	2.86219297987980
C	-3.03431173963773	-2.37896151523409	3.44959320796259
H	-4.50056336792998	-1.12592897060341	0.72462844062366
H	-2.86547586160497	-2.51589862151553	4.50829233670258
C	-2.29768432075178	-2.98707296448122	2.40291852783599
H	-1.47488495060235	-3.67719107035672	2.52783600819418
C	-2.83016529565349	-2.53384867438026	1.16940854609863
H	-2.48825204534400	-2.81523492074176	0.18547278856364
C	-3.89598419201331	-1.64339147314711	1.45422201131696
H	-1.03156262395872	1.57355849491719	-1.42591156493637
C	1.03117954593537	-0.58630467292724	-4.39986229827800
H	1.95669033011822	-0.81165180812854	-3.87192517251567
H	1.28673930762466	0.13010759602790	-5.18414840400719
C	0.48931554051042	-1.83660959895003	-5.01972670458702
H	1.10782503807787	-2.22766142298704	-5.82102891610547
C	-0.61669026177589	-2.48336005248159	-4.67658555399284
H	-0.90511246949398	-3.39142301346669	-5.18808210257242
H	-1.27816660646402	-2.14765001543762	-3.88740754910449
C	2.25531142815094	1.10799206990302	1.60623483210741
O	2.76430665955146	0.85589597770651	2.59722291394503
H	3.72047382808586	3.83496534981548	0.33668815489294
C	2.75017707462451	3.69735231193548	-0.11779210781152
C	1.48800046218660	3.87497791050308	0.52803461175593
H	3.25355581394341	3.14732393757781	-2.20890773666942
H	1.33650258575283	4.20566177398575	1.54544431074022
C	0.47524579320957	3.64684755986026	-0.43266446740664
H	-0.58881721515182	3.72363549556110	-0.25847021005601
C	1.09995924773566	3.30805792895593	-1.65976334691603
H	0.59962297985627	3.09851308463000	-2.59425938808984
C	2.50228394876976	3.35156517901937	-1.46046267603477

[1c]⁺ + CN⁻ (C2-CN, is4)

Fe	1.95079503958104	1.46460438761784	0.25160600713944
Fe	1.38203796622466	-0.77127139900622	-0.66903718559244
C	0.07533801801841	-0.08563406182490	-1.85093489914318
C	2.96237052799709	-2.21793379857660	-0.46602414753769
C	2.12015635330973	-2.55535579157602	-1.54999559766845
H	2.56543935304381	-2.01514320195398	1.70878847533715
H	2.42590088559904	-2.66769502040707	-2.57884210711606
C	0.81575595196499	-2.75604103856214	-1.02952869734353
H	-0.05940704355181	-3.04458117536099	-1.59538971326215
C	0.86206304705846	-2.54905069807415	0.36765954102994
C	2.19210957878203	-2.21500567537117	0.71657944764993
H	4.01938657547328	-2.00125688535654	-0.53096632377841
C	2.57432527803559	0.42605086516420	-1.29937288612047
O	3.40633135373895	0.61989412813525	-2.10509231461762
H	4.36535728046269	3.00376495558601	0.05589383085407
C	3.72215549352805	2.49791716267245	0.76096704880885
C	3.83677221555572	1.15990533683875	1.18974384928469
H	2.26114266462384	4.08764235465283	1.34996000331196
H	4.57832486733939	0.44922676020381	0.85362591382559
C	2.81057521466771	0.90132800303532	2.12965489094440
H	2.64259272472337	-0.02908456885011	2.64501519171626
C	2.05291555891690	2.08265406945253	2.28702659989195
H	1.19293244198878	2.20857757107293	2.92767902149921
C	2.60556698603001	3.06682175471768	1.44091900824077
N	-0.26742385314106	-0.18957580065620	-3.09726225466760
C	0.56655709920552	-0.91460400503397	-4.04947724269608
H	0.47106252658469	-0.45738172499180	-5.03173209569113
H	0.24576590045161	-1.95450755697972	-4.11452959770227
H	1.60554612130669	-0.87352911068439	-3.74467759203179
H	0.02531528796491	-2.62754190549088	1.04352994985511
C	1.40591791877248	2.65032227847601	-0.91335652078405
O	1.20015671173360	3.51629704431489	-1.63129634052624
C	0.26149582738275	0.47015763488591	0.33568897549530
C	-0.76595309704850	0.58775916530836	-0.80517180808894
C	-0.38020356735408	0.39063023013432	1.66485180494097
C	-0.06675333890483	-0.44078035508350	2.77666589215636
H	-1.86940798380967	2.05963117436843	1.52573341345110
H	0.65571766958724	-1.24148979137050	2.78974997255026
C	-0.85584345333309	-0.05163153496864	3.88891161402383
H	-0.83867993984493	-0.50707342438818	4.86908455539484
C	-1.68516561257785	1.01920916756165	3.47818456582682
H	-2.41145359989191	1.53690359491113	4.08916122629320
C	-1.40569881246787	1.28086836050749	2.11397149870644
Fe	-2.07108727012823	-0.64497076179795	2.34611963495826
H	-4.81821197855271	-0.31549968890667	2.92017338663539
C	-4.10002413496581	-0.98410224839358	2.46744325086905
C	-3.39148021250632	-2.01972209283565	3.12888142969560
H	-4.05446992516416	-0.30141219290930	0.34404112192770
H	-3.47412079223627	-2.27798924015452	4.17498032233312
C	-2.54802183937458	-2.64952285760881	2.17968014042654
H	-1.87884554143757	-3.47624343217035	2.37249834817762
C	-2.73708239296242	-2.00583419687325	0.93020701482989
H	-2.24660217288486	-2.26729866162419	0.00259082948410
C	-3.69422052486577	-0.97456072361732	1.10939284473680
H	-1.59738160083065	-0.10393305757090	-0.59763911950989
C	-1.39884315393379	1.88037601033647	-1.05658349463941
N	-1.91434830075517	2.90055077795228	-1.19986943632556
C	-1.51486320359395	0.31189978731198	-3.66651017485635
H	-2.25713053738593	0.44840789999497	-2.87950556964728
H	-1.91949931475095	-0.47318053262351	-4.31196504951983
C	-1.35812233937844	1.57468049666088	-4.45440615685041
H	-2.26735177725735	1.89986846765718	-4.94865111394414
C	-0.24740901807879	2.28571478325427	-4.58485385914015
H	-0.23619758800822	3.19135672045471	-5.17536855703781
H	0.68613848132450	2.00686626841314	-4.11199676646359

[1c]⁺ + CN⁻ (C2-CN, is5)

Fe	1.91700633439097	1.42618226976848	0.21743675981620
Fe	1.34552570739920	-0.83291472932694	-0.65083981570828
C	0.05541953928273	-0.11777528066248	-1.84703700085749
C	2.90031134207225	-2.30498340380622	-0.49803475450890
C	1.99025662769158	-2.65070281775344	-1.52209366619449
H	2.63073592772374	-2.02685575319156	1.69107903201115
H	2.22723501334766	-2.79703895905192	-2.56539856244899
C	0.71451522685141	-2.81155821460170	-0.92143420930029
H	-0.19519641143183	-3.09728017457127	-1.42957125858966
C	0.84622723287593	-2.57109356424752	0.46380914836529
C	2.19907255228209	-2.25162781776474	0.72793059727173
H	3.95580390822024	-2.11141619043782	-0.62869490961948
C	2.56471898481724	0.33266969491565	-1.28356089794271
O	3.41712522673476	0.50190866128362	-2.07414302577750
H	4.30362983279307	2.98903459540139	-0.05377192197210
C	3.67406789695732	2.50048036948621	0.67543094869090
C	3.81225499714466	1.17998415911372	1.15019979848869
H	2.19357980166587	4.08839920512414	1.21966531100511
H	4.56090363368767	0.46771181997138	0.83338757836984
C	2.79720699540440	0.93930596260327	2.10702029266888
H	2.65187944075724	0.02521803989378	2.65847730001054
C	2.02376155020312	2.11493443937765	2.22950656824700
H	1.16788553562992	2.25184681639333	2.87347157697734
C	2.55416229189728	3.07678742801377	1.34401080849930
N	-0.23291640127504	-0.10753837445249	-3.11018755903091
C	-1.42880226046307	0.51214882709392	-3.68517117397390
H	-1.63669188410837	0.05014462207819	-4.64644495406331
H	-1.27334143780158	1.57914543877322	-3.83642426214915
H	-2.29421338295615	0.35498594545236	-3.04701766151064
H	0.04678183039004	-2.61953659539847	1.18524531693915
C	1.35601063993858	2.53834121589071	-1.00988417788629
O	1.11909724932128	3.33837005948775	-1.79222630085269
C	0.23218549156397	0.42376942753692	0.34285557665638
C	-0.80322925100266	0.51924964707846	-0.79363907923805
C	-0.39187072472179	0.37656655792278	1.68196343786868
C	-0.05428372969890	-0.42314637111072	2.80986758763530
H	-1.89531728840248	2.03257614045143	1.52733282782957
H	0.67912884914852	-1.21365678195428	2.83402642865305
C	-0.83077702578936	-0.01408813694955	3.92353172552569
H	-0.79577563062251	-0.44595831466087	4.91379083479955
C	-1.67438064034632	1.03985600018495	3.49934152672559
H	-2.39626218603806	1.56646807509400	4.10792320692655
C	-1.41683345715146	1.27071555068352	2.12527769645915
Fe	-2.06345142162170	-0.65233084855544	2.41034283034098
H	-4.80876067534427	-0.31241531441605	2.98233558089643
C	-4.09019041887469	-0.99325780291752	2.54885675581902
C	-3.37615502107833	-2.00508177564826	3.24044861787159
H	-4.05244245885616	-0.37768814143685	0.40431774977759
H	-3.45421377991252	-2.23018884367355	4.29453007509951
C	-2.53376102218285	-2.66220940144400	2.30898075034048
H	-1.86078037868374	-3.47981751748554	2.52562655947295
C	-2.72843892978550	-2.05849805335165	1.04044004315929
H	-2.23846280342972	-2.34468337846977	0.12008260293761
C	-3.68814154916413	-1.02501097437493	1.18986279109702
H	-1.61578280427111	-0.19657646372481	-0.59447525952406
C	-1.46316361620212	1.80266681849421	-1.03096347452206
N	-1.98656249382870	2.81964005116063	-1.16887323729778
C	0.65558552044671	-0.72466906129305	-4.08746882851106
H	1.64690775604169	-0.82492015161460	-3.65043319543172
H	0.75984813715499	-0.03144221032509	-4.92723382314185
C	0.17959732318888	-2.05033489432331	-4.59126695541137
H	0.79666874034316	-2.46507034235457	-5.38182531294752
C	-0.88378892654048	-2.72265042253286	-4.17089608996741
H	-1.14083875969271	-3.67979291666464	-4.60339195364252
H	-1.53736036608984	-2.35591284418095	-3.38855092123090

[1c]⁺ + CN⁻ (C2-CN, is6)

Fe	1.57389268152132	1.59631004868883	-0.02020004733098
Fe	1.27706061063024	-0.75742901771705	-0.81938982737823
C	0.00887447409588	-0.10660957929444	-2.07406857734516
C	2.88315739114017	-2.20174153586995	-0.68920637915665
C	1.96301358237451	-2.56294348750140	-1.69391575515506
H	2.64838642404529	-1.93651628581084	1.50994586104029
H	2.18137117449387	-2.70268976575681	-2.74192461745660
C	0.69770343832885	-2.74428054224084	-1.07009831486641
H	-0.21496110588604	-3.05126076626417	-1.56083671688761
C	0.85485992459316	-2.50231544537801	0.31181460190944
C	2.20392227240707	-2.15593360900192	0.55155805566176
H	3.93291403926431	-1.99392927779279	-0.83929409292182
C	2.54328486998365	0.45017539458814	-1.28780311491618
O	3.50315336477630	0.60195811516761	-1.94283040241874
N	-0.20554274405571	-0.08267508005614	-3.35169061139616
C	-1.42715295157532	0.41609571878647	-3.98615955087656
H	-1.51872679178523	-0.02690090828751	-4.97434081315306
H	-1.39178492457008	1.49900299183425	-4.09387103601752
H	-2.30623495998384	0.13300483465478	-3.41388789016208
H	0.07314215544862	-2.56174924893751	1.05084996312427
C	0.03106025293872	0.37986040232793	0.13218796213021
C	-0.96905866027613	0.38545875205002	-1.04481303867922
C	-0.60267468133714	0.31577027536312	1.46423162728487
C	-0.17196943697826	-0.38241856431734	2.62965573838523
H	-2.31772024303961	1.74482269474135	1.23520022675558
H	0.65788894571156	-1.07015146754215	2.68763894257396
C	-0.99731705452263	-0.02094218879868	3.72490563938242
H	-0.90735634078245	-0.39220585402209	4.73603530702685
C	-1.96529464592107	0.89654899347158	3.25307365632540
H	-2.75085336247707	1.35566097307186	3.83675140942207
C	-1.73556058402440	1.09104348713980	1.86783714487412
Fe	-2.14144747715781	-0.87696366316916	2.25278696845931
H	-4.87372538049188	-0.86560553383059	2.96546692740532
C	-4.10251466198708	-1.45582842117916	2.49140220553224
C	-3.23932205056159	-2.37524921601859	3.14124161231381
H	-4.24011302806111	-0.83465698280249	0.35184436839539
H	-3.23893654686985	-2.61042131343541	4.19603794434025
C	-2.37431537594102	-2.92965132952702	2.16526228172342
H	-1.60621848104689	-3.66855348732681	2.34602862422293
C	-2.70232499406838	-2.35214156573679	0.91140878316873
H	-2.23523569937403	-2.58269128407314	-0.03588810172732
C	-3.76781111192473	-1.43871027896393	1.11357882526554
H	-1.68584144280217	-0.43718671688615	-0.88979663381208
C	-1.80771336943469	1.55672647619674	-1.30824871225396
N	-2.49187324721872	2.46693692110854	-1.48579996471362
C	0.80515283126727	-0.56047587514182	-4.28695216275280
H	1.76708163802072	-0.58846021057519	-3.77786422559874
H	0.90059076842130	0.18116996009961	-5.08549968730167
C	0.50421745905544	-1.89990885780634	-4.88166488754267
H	1.19887781040308	-2.19810686163201	-5.66033951968909
C	-0.48733143781772	-2.71442185893130	-4.54657799430158
H	-0.60772997818241	-3.66958559331191	-5.03914350208346
H	-1.21334201829938	-2.47415001934388	-3.77930404791168
C	2.38159145331284	0.97882698740616	1.40855470801964
O	2.96005269766494	0.68115002668441	2.34893166926597
H	3.64302103396464	3.57163992523639	0.39602833834128
C	2.62727955698861	3.44363386359802	0.05103930357725
C	1.44860136316868	3.49709234021516	0.85523894830427
H	2.88238720663182	3.15944982483800	-2.13076681608204
H	1.41096446737810	3.67182671018230	1.92112769416204
C	0.33858189743798	3.31310451430282	0.01099065151335
H	-0.69060326528131	3.32252011304110	0.33194681412026
C	0.81336612010800	3.14256740409649	-1.31796331704863
H	0.21849257542697	3.03509683493244	-2.21187129000081
C	2.22263857273186	3.24031111045751	-1.28006615508918

Compound 3

Fe	1.30324899196148	-0.19634152529638	-0.20066958075996
Fe	-1.18917320451761	-0.40665942537738	-0.10536137535141
C	-0.06190777279345	1.05076304149407	0.55101289505504
C	-1.69709695162661	-2.41418320000489	0.42305235572355
C	-2.81952640740777	-1.78029904479687	-0.13626841714154
H	-0.51422474548576	-1.96265810706634	2.25504338286549
H	-3.35317403054094	-2.09477724690943	-1.02101880324848
C	-3.15106955534339	-0.67456864342308	0.70381870940484
H	-3.97998316987276	0.00465363680884	0.57039174769240
C	-2.23830775951116	-0.63935985993497	1.76551699594974
C	-1.31150383808651	-1.69577802749085	1.58137285138569
H	-1.20038751976528	-3.28967535219089	0.02955881561801
C	0.07162294669065	-1.12517230106899	-1.31109853316498
O	0.09375824782830	-1.83292726267585	-2.23929206563988
H	4.09992818973464	0.22864807492010	-0.59511259278955
C	3.39081953254979	-0.36620712059931	-0.03588652213146
C	2.86091874720081	-1.61527079402378	-0.43917301141712
H	3.07021638061924	0.85290201709496	1.80603561346880
H	3.08625548134075	-2.13611468583255	-1.35791810225832
C	2.00020924125100	-2.06220105439307	0.59338753171263
H	1.44242503351841	-2.98794138014776	0.59429531618666
C	1.99862914282739	-1.09525894132947	1.61918766070034
H	1.45655400025393	-1.15135439715693	2.54881647813911
C	2.84806145393655	-0.03307387496961	1.23017806419903
C	1.64455002385588	1.02273317189307	-1.42665920127095
O	1.99437066459390	1.80352664535789	-2.17954304791902
C	-1.47042240200705	1.27977768718558	-1.74316686198808
H	-0.63061287235668	1.18679445396845	-2.42307153285196
C	-2.52160505942912	0.46394959616863	-1.93337804016454
H	-2.51388907932371	-0.28118376340654	-2.71846215713565
H	-3.47547854575309	0.65037325678340	-1.45921215950269
C	-1.44477345085596	2.45624267388438	-0.82568629332168
H	-2.37406735325996	2.49714338902594	-0.23384850075015
H	-1.40224013852667	3.37599891157277	-1.41944418717286
N	-0.26049490483656	2.36486067819424	-0.01366350709863
C	0.01273490183738	3.53867882472207	0.77781124703056
H	-0.71065105786217	3.71131912469159	1.58667006916308
H	0.00033077818580	4.41723537683980	0.13127500629336
H	1.00613856004222	3.47651199311445	1.22191637964933
C	0.08223977887080	1.12962204862110	1.97210777703277
N	0.20716993786504	1.20562945715312	3.12324123651448
H	-2.23740921580173	0.07414694860047	2.57509335929399

FcCCH

H	-0.20182957161121	2.17430400426056	2.06803644991517
C	0.10465495403287	1.14668904996766	1.93424851654109
C	1.32255136417712	0.71009776080158	1.35431131947942
H	-1.62963977020139	-0.00185760877239	2.74369513989209
H	2.10445024814830	1.34597136070438	0.96417232729801
C	1.32358019947330	-0.70837510899477	1.35374373568717
H	2.10639588885233	-1.34280847475912	0.96309124664570
C	0.10632866222089	-1.14721794017449	1.93332128658684
H	-0.19866021852498	-2.17538748653355	2.06626185159106
C	-0.64823069693982	-0.00095905758109	2.29172243276666
Fe	-0.27321250692194	0.00014807322999	0.26634393420786
H	-0.34365668555013	2.17823815755706	-1.52916563097907
C	-0.65346049706717	1.15285422821896	-1.38856503033903
C	-1.87458684228253	0.70986289860231	-0.83261618647325
H	-2.66474959592245	1.34474626647761	-0.45907612397398
C	-1.87515816647215	-0.70854147268062	-0.83245680661801
H	-2.66583899362597	-1.34270350556549	-0.45878761706637
C	-0.65438987492459	-1.15265167892215	-1.38829962496995
H	-0.34540923280474	-2.17831634553258	-1.52865946650326
C	0.11017512831652	-0.00024757991150	-1.74048604694371
C	1.41049400911262	-0.00082291275470	-2.31012125208915
H	3.47642215547939	-0.00171920611175	-3.24946609979721
C	2.50565004303575	-0.00130242152589	-2.80998135485810

[1d]⁺ + CN⁻ (C1-CN, is1)

Fe	1.81240245985935	1.39066768339583	0.13535783054116
Fe	1.33235387089745	-1.01896057304311	-0.48603741568227
C	-0.01998406582840	-0.51281325444408	-1.94335029758256
C	3.03475300944032	-2.25528176727944	-0.46815241298889
C	1.99475927644620	-2.86320529582764	-1.20237880294813
H	3.16789372622391	-1.64473964848140	1.67309820276918
H	2.02414111407469	-3.13098620474483	-2.24869134202869
C	0.89825989628084	-3.04605864152921	-0.32209367043125
H	-0.05154828151104	-3.49379119673226	-0.57545957511263
C	1.27475921981890	-2.56660821965326	0.95585613255407
C	2.58792772453829	-2.06890825112777	0.86833025368779
H	4.01174122221312	-1.99577962448683	-0.84823610675687
C	2.49551376530500	0.31110489267922	-1.25537102373537
O	3.33452422192923	0.37510510463582	-2.05642166299049
H	4.16292031710502	2.94739192067326	-0.38813892185014
C	3.55745986715984	2.55106550148985	0.41332232289114
C	3.72538867801055	1.30448949644509	1.05557145924254
H	2.06926017549514	4.17425761003474	0.77778898118497
H	4.48423828122266	0.57022303422475	0.82364269114231
C	2.73174833778275	1.17584080096027	2.05413847552586
H	2.61887577622278	0.34337915116077	2.72901059987012
C	1.94108335156792	2.34601670409962	2.03641100542063
H	1.09691664172051	2.56020514357351	2.67451460036366
C	2.44832318097702	3.19271884465856	1.02607563008376
N	0.20637421280941	0.53049604383984	-2.90543051354509
C	1.08505410168583	0.14517581398519	-4.00795501204635
H	1.74805998568104	0.95914365044239	-4.29745080401787
H	0.51406069892513	-0.16163762414725	-4.88947922652240
H	1.70595059032382	-0.69427418784963	-3.71068075501018
C	-0.62816740925907	-1.66129583296345	-2.57804458777122
N	-1.07696284199491	-2.56320678531574	-3.14355949570030
H	0.64612963969554	-2.56537301870812	1.83455104894094
C	0.92594946827807	2.42740032062764	-1.00050071198366
O	0.39395660723161	3.25931729909144	-1.56463098166777
C	0.16880760187395	0.40018131011029	0.38498452434579
C	-0.52880258273010	-0.28178923191236	-0.608275524445482
C	-0.50714539554726	0.52352653606467	1.68926927663328
C	-0.13523428848308	0.02661230705274	2.96683353442862
H	-2.14588181218120	1.91542499895792	1.10302638778893
H	0.66930738390440	-0.66427522499026	3.16988261257617
C	-0.99756765617514	0.59042877455077	3.94114809786249
H	-0.96793578397496	0.39339473503976	5.00346051171502
C	-1.92209148908381	1.43003871704592	3.27285844868868
H	-2.72006862894030	1.99475969931772	3.73355553264378
C	-1.62929320933310	1.37829469422621	1.88684599035470
Fe	-2.08886451122904	-0.49760557698556	2.59049209963341
H	-4.90478724646090	-0.29691537160730	2.72257872660599
C	-4.08852390747346	-0.99670370484949	2.61438841024244
C	-3.40724023204328	-1.65181944279064	3.67175085901177
H	-3.79488761562352	-1.08732443873198	0.40434254626107
H	-3.61322484765422	-1.53713891843205	4.72642925166666
C	-2.39971330641053	-2.47175132490378	3.10419577905504
H	-1.70617408298676	-3.09582808542019	3.64959425378258
C	-2.46021955678799	-2.32572718880758	1.69576963306940
H	-1.82848943258613	-2.82883214951605	0.97848840662911
C	-3.50247742225768	-1.41258347448517	1.39282129176637
H	-1.39384428751317	-0.86707372111815	-0.30590306953826
C	-0.90349072095319	1.30344006814953	-3.30407742214782
C	-3.05013307034563	2.95698698042979	-4.12953584911814
C	-2.15830853618789	1.23060216616300	-2.69024287425208
C	-0.76510551409338	2.22249387360257	-4.34573341242437
C	-1.81193470738738	3.03659341888243	-4.75626779657596
C	-3.20506212136320	2.04143659227915	-3.09306078569723
H	-2.35092093370657	0.53813393081172	-1.88486693872174
H	0.18106956941926	2.33242471373284	-4.85706107243974
H	-1.63181198027981	3.72860364293686	-5.56798245327194
H	-4.16420017364666	1.95485596945791	-2.59733911271315
O	-4.12936174958836	3.70470897101766	-4.45191042845440
C	-4.00622820866594	4.62161543885076	-5.51530834505016
H	-3.25229860093264	5.38817843716504	-5.31314999203630
H	-4.97382290974661	5.10614224220084	-5.62372543488303
H	-3.75521585315319	4.12708074682068	-6.45843757682813

[1d]⁺ + CN⁻ (C1-CN, is2)

Fe	1.74303404623674	1.73035720266544	0.51115548392365
Fe	1.33068852929225	-0.52418511896408	-0.57382000582167
C	-0.07367991696688	0.24265366075386	-1.84639990232336
C	3.06181419519576	-1.69689415859046	-0.81133914803102
C	2.02697196905820	-2.17996979396587	-1.64042067139130
H	3.19988901071899	-1.49818494745954	1.40868974511209
H	2.05366057464442	-2.25055714952762	-2.71805926254765
C	0.94503527967963	-2.55243301768535	-0.80425543590007
H	0.00277960010225	-2.96586776266764	-1.13355453513558
C	1.32652297335528	-2.31681326995387	0.53914255512051
C	2.62813680452543	-1.78288012683646	0.53953604507724
H	4.02768627023834	-1.34421387708090	-1.14196423777765
C	2.43811307218781	0.96102528791337	-1.08011141581165
O	3.25660519947735	1.21525575558743	-1.86121290173169
H	4.01319555605090	3.47026137669362	0.26218090395190
C	3.45002003486762	2.88865599670796	0.97691598716747
C	3.69043522228634	1.54720453180987	1.34649481641274
H	1.91292082453811	4.33339264392108	1.70861896118800
H	4.46839862155652	0.91152656150837	0.94718030007930
C	2.73741906116111	1.17087864603731	2.32111752753033
H	2.68059132725813	0.21396591850042	2.81281962742396
C	1.90172903335029	2.28293047927587	2.56494424772166
H	1.06940433049590	2.31892939656808	3.25156207647893
C	2.33888355812346	3.34032149585330	1.73860156984162
N	-0.02172091116899	1.54054061355302	-2.46072765969721
C	-1.35892379900041	2.11681214305443	-2.60956429430260
H	-1.93982612823675	1.61197412718596	-3.39074038422188
H	-1.30715233440884	3.17170611517403	-2.86390343113386
H	-1.90276860641302	2.03378984241060	-1.66995792753195
C	-0.68076566691163	-0.75438048519570	-2.70410128304817
N	-1.15149422875552	-1.53591867579960	-3.41273046981612
H	0.70231519378098	-2.47916037194974	1.40490977752882
C	0.79598906647086	2.94623044959374	-0.37875314773053
O	0.24183028922094	3.88510245413245	-0.71012868307904
C	0.14010872572901	0.64181345599986	0.60803224754708
C	-0.56116720609462	0.13727830025482	-0.48150923554410
C	-0.48731200026879	0.46386052288398	1.93155699894229
C	-0.05025476933876	-0.26602130968768	3.06929286960298
H	-2.20072725727940	1.86598398489076	1.68738863481120
H	0.79255431406267	-0.93967717189353	3.10791744491005
C	-0.89953260271480	0.04642913070558	4.16173991288468
H	-0.82156100264475	-0.36025472029815	5.16006448478444
C	-1.88029954416640	0.96012367286923	3.70483162938790
H	-2.68374570725427	1.38129839582909	4.29219099887467
C	-1.63547361935666	1.20556357435254	2.33042934065161
Fe	-1.99329876753829	-0.79588388141673	2.64794845867467
H	-4.80641946872781	-0.76594928284381	2.90835705869719
C	-3.96675396569549	-1.38795237687616	2.63318476619853
C	-3.21430267702559	-2.20950406197827	3.51109238862850
H	-3.76676911777277	-1.01541330534879	0.44205441169503
H	-3.37809826427158	-2.32024634865913	4.57360272811487
C	-2.19919692262395	-2.84671360761932	2.75458460445451
H	-1.45555743056554	-3.53237632323510	3.13503208368864
C	-2.32786842091893	-2.42188474716806	1.40870633293947
H	-1.71159723806434	-2.74262463052917	0.58131111442113
C	-3.41765268974596	-1.51799318215069	1.33295012201865
H	-1.39416071108586	-0.53473398481561	-0.29319361791173
C	0.80754553657773	1.74184455277362	-3.59124032515102
C	2.42971611348015	2.26630673029602	-5.84517205970453
C	1.47276101371187	0.71365827375558	-4.26103102300116
C	0.99606606283201	3.03747231114417	-4.07013491477219
C	1.78574097887083	3.30477575801294	-5.17926061688144
C	2.27092862269629	0.97072582755245	-5.36223155865645
H	1.39601479908591	-0.31031372081723	-3.92780867247413
H	0.53190668798987	3.87613740041265	-3.56878609411004
H	1.88922575139367	4.33298241973746	-5.49896941472484
H	2.77285343743135	0.15077131759714	-5.86109555533100
O	3.21052707216985	2.41986452370787	-6.93676335173595
C	3.37358165524850	3.71793416125024	-7.46246560362142
H	2.42205080288560	4.15874774683864	-7.77386681447445
H	4.01464875409371	3.62227393356282	-8.33585391824912
H	3.85455300288389	4.39452071768648	-6.74996468310968

[1d]⁺ + CN⁻ (C1-CN, is3)

Fe	1.42827051238669	1.92474875201862	0.45905174678900
Fe	1.314113073575983	-0.41300798215583	-0.62277787103843
C	-0.04622764313420	0.26672666621805	-2.00306225667609
C	3.11180299007762	-1.51549249135215	-0.84195576063051
C	2.10608520625649	-2.04995885454892	-1.67054225698279
H	3.24376244700748	-1.32959830436419	1.37820834496530
H	2.14225651631863	-2.13162401040534	-2.74727801118083
C	1.03357442089549	-2.45833315429653	-0.84052409725499
H	0.11595629342193	-2.91802453864044	-1.17729624776028
C	1.39671825194116	-2.20044038664332	0.50489955005460
C	2.67538497386108	-1.61631705947999	0.50814943557733
H	4.06673134661930	-1.13283540521354	-1.17026573465544
C	2.43191773193593	1.15840196756259	-0.96748826022208
O	3.30739552381862	1.44069968133049	-1.66675078047079
N	-0.03394849919843	1.54771166239857	-2.64830898983282
C	-1.32817002465700	2.21338094175081	-2.68546620402372
H	-1.88042800098680	2.00093451562596	-3.60822881661089
H	-1.22522251323905	3.29499771222526	-2.59783636883019
H	-1.92998512709391	1.88112145993062	-1.84445259625773
C	-0.51153304785078	-0.76533690124814	-2.90631309335856
N	-0.86953148440784	-1.56423126524214	-3.65991704185855
H	0.78028388771851	-2.39137714702369	1.37060774540904
C	-0.02860803042050	0.64317949713230	0.46567716683398
C	-0.62529495819477	0.12693790955992	-0.67681055285972
C	-0.72115125801610	0.43329060907546	1.74876662623889
C	-0.26901977363291	-0.19358529274281	2.94297431557723
H	-2.56939118580542	1.61654665586693	1.35375501155149
H	0.63653192649025	-0.77071841246698	3.05783294339469
C	-1.21384006530223	0.05496383124614	3.97070300387081
H	-1.14943205137379	-0.30124067165305	4.98904984193515
C	-2.26566730352747	0.82781881712266	3.42092176341628
H	-3.14421948802412	1.17510784968497	3.94579750311663
C	-1.96976014555271	1.04959766205496	2.05279213391960
Fe	-2.11562211851630	-0.96068102947922	2.43189676227931
H	-4.90128059838047	-1.30552880135294	2.73445793135857
C	-3.99331183016185	-1.80312001601588	2.42513291705407
C	-3.12707830260394	-2.55142445300179	3.26302697421444
H	-3.87579429740076	-1.32583963492788	0.24753043830555
H	-3.26021182269145	-2.72458870590659	4.32140645915907
C	-2.05116204011356	-3.02412019724197	2.47039394571238
H	-1.22083410996341	-3.62290015726923	2.81691220348558
C	-2.25486468683931	-2.57086053787929	1.14286657565357
H	-1.60792044914619	-2.76634502573204	0.30137216664543
C	-3.45352235587002	-1.81352689457278	1.11444079375651
H	-1.43350799322359	-0.59043153557115	-0.55204790784600
C	0.77256802095539	1.74423556885637	-3.77405247394224
C	2.37721414656786	2.19527234191448	-6.06901865402372
C	1.74104561040508	0.81892469837988	-4.18690616999591
C	0.63908743969556	2.89778565848932	-4.55109920179661
C	1.42613281377082	3.12589621682459	-5.67492222990898
C	2.52397738484920	1.04079467318614	-5.30310592467992
H	1.90169292533179	-0.09259531710595	-3.63291475649755
H	-0.08990148487318	3.65552725892528	-4.30085429284235
H	1.26637371631838	4.04110637377408	-6.22916357305160
H	3.25863403105039	0.29872699223706	-5.59159133919827
O	3.17868729914332	2.31658458796788	-7.15262017162402
C	3.03848440672454	3.46775898054089	-7.95267138625068
H	2.03456375059680	3.55438990691550	-8.37909178404338
H	3.75332334338488	3.37142466343669	-8.76696225282754
H	3.26172658182926	4.38517805646134	-7.39959935058244
C	2.29715235126092	1.20429458118734	1.82152580095847
O	2.88148883995535	0.87029051218590	2.74031487679983
H	3.26187773086934	4.03583912436105	-0.32809809860556
C	2.26284925970804	3.84800520468719	0.03658743797200
C	1.87404759394493	3.78538563797865	1.38728051821668
H	1.06631883424814	3.69905685107112	-1.83669987596875
H	2.52995258131730	3.89815922518357	2.23946491951498
C	0.48233028334208	3.51710233411528	1.44207966079513
H	-0.11347525232255	3.41439292384848	2.33695807839858
C	0.00619780192575	3.47085320275968	0.10516181050861
H	-1.02055649532940	3.31306042550316	-0.18570107774040
C	1.09638292614986	3.67047099193840	-0.75931994150830

[1d]⁺ + CN⁻ (C2-CN, is1)

Fe	1.83349457977278	1.26600505619815	-0.06242024582784
Fe	1.59454791633626	-1.05969060520085	-0.83485076261562
C	0.15892269290954	-0.65219998166843	-1.97508202813074
C	3.40772975839716	-2.09349951813120	-0.32390713344377
C	2.92250897589335	-2.55622223609406	-1.57669687341401
H	2.48879442640267	-2.09272002893407	1.70198417192411
H	3.45470051096233	-2.52351205046550	-2.51635747823125
C	1.63878393588955	-3.10064174270611	-1.35957525967952
H	0.99944135349913	-3.54061621937514	-2.11243444255950
C	1.32197936495263	-2.96559882585537	0.01280418631002
C	2.42567398293316	-2.34298078188113	0.65307388648948
H	4.36610753715819	-1.62232874428096	-0.16114267147548
C	2.42607811791860	0.32434879619628	-1.66088996365088
O	3.06216552559185	0.62790826519545	-2.60039679871040
H	3.11408189348048	3.79710130136080	-0.29649142752972
C	3.06305963589111	2.92128418468888	0.33477538666024
C	3.88249703394816	1.78438267859794	0.23920961477568
H	1.42454708641637	3.42994827397734	1.77147815746672
H	4.66794199835875	1.62587140998197	-0.48480706922266
C	3.50455164554576	0.88284815055455	1.27101110401571
H	3.96796102039349	-0.06669421124727	1.48343078141022
C	2.46307351797937	1.46898264573876	2.00628693942146
H	1.96470553609780	1.02278678938185	2.85167437016993
C	2.15724789658011	2.71829939033552	1.42061553803175
N	-0.19078990587064	-0.70788452638884	-3.22267005762435
C	0.70399980381905	-1.20778670631966	-4.26061097952241
H	0.83640502346199	-0.44170181552825	-5.02285201305898
H	0.26872846779674	-2.09139909049844	-4.72613909536504
H	1.66536938048009	-1.46327654515578	-3.83075467566399
C	-1.59667585815982	-1.35649546616677	-0.65621976809201
N	-2.18170529980671	-2.34446879238516	-0.56709550255123
H	0.41723612561037	-3.31719524891552	0.48290366800044
C	0.75577033414784	2.23770675804941	-1.01896351792866
O	0.05405455288711	2.94289295018296	-1.58669095963007
C	0.30355159822924	0.00803214967711	0.20086636291029
C	-0.77467900922661	-0.16973927300768	-0.89306597286522
C	-0.22808167668972	-0.05929436709141	1.59521281677356
C	-0.47003407939563	-1.20514327035401	2.40437367267830
H	-0.40888772650803	2.10000871483226	2.11798445439122
H	-0.39388482190052	-2.23188623409737	2.08239572055684
C	-0.78325929710886	-0.78917198554020	3.72528822053764
H	-0.99112115537331	-1.44066688550246	4.56258227492355
C	-0.77847614960109	0.62695052057096	3.74477617481091
H	-0.99199984759763	1.25603819733803	4.59760503208876
C	-0.48489372482542	1.06911899467879	2.42966128305449
Fe	-2.19828894271048	-0.03436871837053	2.45475711489435
H	-3.65571348117933	2.30522919479441	1.81442226052631
C	-3.75550654303137	1.25107801374954	2.03037350986932
C	-3.92453402114900	0.67613790091379	3.31477704297524
H	-3.64756978049865	0.31996030459628	0.01033658850977
H	-3.96797250622723	1.21451829415254	4.25093461100114
C	-4.00955416586029	-0.73100648284717	3.15769265129759
H	-4.13466436481895	-1.45158443870977	3.95346704094603
C	-3.89067081525301	-1.02583792228303	1.77863887407255
H	-3.91016949192497	-2.00972610176720	1.33625959470496
C	-3.73616671808608	0.19956557919061	1.08002914318555
H	-1.45730760058122	0.66477040904035	-1.11774389029833
C	-1.49413336090946	-0.32567983144916	-3.68866879394776
C	-4.01008262044723	0.38491450229917	-4.63593989847652
C	-2.47375472051315	-1.29835401173408	-3.85267987502565
C	-1.76548111966973	0.99114327395031	-4.01038367650404
C	-3.02087797220643	1.35435728311340	-4.48036064774602
C	-3.72336531488508	-0.94624102017168	-4.32037932754749
H	-2.26156886146297	-2.33167771768500	-3.61044721073349
H	-0.99835834389298	1.74611352840040	-3.89887223632782
H	-3.20250772597860	2.39284926876236	-4.71974770039588
H	-4.49026622903070	-1.70007979309971	-4.44405282203314
O	-5.25197745786335	0.63271589510676	-5.07914631662173
C	-5.59995348238958	1.95838266059411	-5.42191810281682
H	-5.51231817422045	2.63697254073666	-4.56956768850333
H	-6.63827526952818	1.93119795227896	-5.74255507516486
H	-4.98827559335844	2.34160036169232	-6.24298429044783

[1d]⁺ + CN⁻ (C2-CN, is2)

Fe	2.00305159498753	1.54455769337646	0.01368671580023
Fe	1.42679767928538	-0.70834801251732	-0.87854720331519
C	0.27594601377664	0.04246815791840	-2.16314882350623
C	2.94298871252414	-2.21368264340661	-0.63878226713694
C	2.06194241735296	-2.55834815677097	-1.68521154339860
H	2.60743504821221	-1.87632467109040	1.53356342858548
H	2.33359600969912	-2.72067227873508	-2.71741913070393
C	0.75876398187344	-2.66483008193416	-1.12717071440235
H	-0.14401162500641	-2.93723958072981	-1.65538055946242
C	0.85092353676787	-2.39511295386021	0.25837048051475
C	2.20152356042168	-2.11006305422830	0.56154027984882
H	4.00713681702274	-2.05090014038201	-0.73719185610304
C	2.71083662988717	0.42855029841236	-1.43836605204149
O	3.62104259313299	0.57005620970221	-2.16602382297517
H	4.38831844578617	3.11494274686903	-0.20432701750256
C	3.74287645953134	2.62892880661996	0.51263136179946
C	3.87743201302831	1.31450697564384	1.00356182731357
H	2.24273236537337	4.21461402207557	1.00808053384556
H	4.64011224684863	0.60491997227584	0.71578297387335
C	2.84036429336346	1.07684496636369	1.93584461845142
H	2.70055447576195	0.17159265760637	2.50193833317418
C	2.05490093613258	2.24763526589510	2.02653827424055
H	1.18140730966749	2.38501702423570	2.64579798462611
C	2.60382946344008	3.20514968426433	1.14825437883150
N	0.05177718940328	0.01850720433585	-3.44219644186137
C	-0.97293290273960	0.79003514095482	-4.14379569283731
H	-1.78519108286643	0.13744331354660	-4.46206669154653
H	-0.52489767076260	1.24694174094884	-5.02402102903432
H	-1.37171886765821	1.57832999732464	-3.51326965741443
C	-1.91130973485850	0.14142638570915	-1.27789868157762
N	-2.92145134666419	-0.37218562418860	-1.48205438401876
H	0.02770572936003	-2.38470012265593	0.95378733121543
C	1.46795334927350	2.67006318094451	-1.20798386053578
O	1.19154875360520	3.48152535211835	-1.96688405801701
C	0.26756264925114	0.55816843014158	0.02694248414991
C	-0.61575063380208	0.81476717568688	-1.20884604403687
C	-0.43300667777577	0.54159463103251	1.32254323616181
C	-0.02783388331580	-0.08437567966740	2.53606833403477
H	-2.09126573697290	2.00133205990219	0.97044039342893
H	0.77099403730833	-0.80267801118011	2.63600049153687
C	-0.79850815421846	0.43061359756008	3.60912011044147
H	-0.70042357438990	0.15821783268412	4.65083889689841
C	-1.74238443218507	1.33660117257402	3.06544236084212
H	-2.49209253314284	1.88740356338976	3.61614533307919
C	-1.53739502813938	1.38045480733935	1.66210088320319
Fe	-2.01261166844665	-0.53969908453126	2.29502065416150
H	-4.61250822233126	-0.46102821954774	3.39608715502850
C	-3.91339337236872	-1.09274440072560	2.86663290975671
C	-2.95334059411592	-1.95131567685998	3.46008746768331
H	-4.36876954761450	-0.66075128686751	0.72716733556355
H	-2.79157607580166	-2.08907296722490	4.51978323335226
C	-2.23547728830048	-2.58949399449250	2.41806841720384
H	-1.43734123500827	-3.30679553032864	2.55008923092931
C	-2.74708036401433	-2.12283173432583	1.18127866052973
H	-2.40701381934867	-2.41824645353693	0.20059442849034
C	-3.78374874637417	-1.19541899740981	1.45952929365408
H	-0.83680938976858	1.86266361239047	-1.45762803036907
C	0.80296395533265	-0.86974306817657	-4.27998484740484
C	2.23224316318435	-2.61908768700383	-5.89913779579909
C	2.00277094850857	-0.46204036550801	-4.84496737116036
C	0.30524654081002	-2.13214023533151	-4.54370002040296
C	1.01358435165262	-3.01353079188520	-5.34931829023607
C	2.71699247277704	-1.33307148024511	-5.64422554592353
H	2.38544789909670	0.53086523465636	-4.65247641681692
H	-0.63492437020960	-2.44402576510880	-4.10605162844434
H	0.60380756465463	-3.99805684013348	-5.52766352188376
H	3.65932619866223	-1.02505993285794	-6.07896873942640
O	2.99835824268838	-3.39702921007751	-6.68101968985654
C	2.56467634886598	-4.71142722019101	-6.96480367295351
H	2.46989628593946	-5.31544212405940	-6.05840576697437
H	3.32517022206759	-5.15608402300882	-7.60177865308200
H	1.61054507188179	-4.72192581371394	-7.49845931008831

[1d]⁺ + CN⁻ (C2-CN, is3)

Fe	1.70256378821302	1.66821241695489	-0.35804105754100
Fe	1.32403217728854	-0.70838538095251	-1.03998640789539
C	0.15123981086707	-0.05178420822089	-2.35519719729806
C	2.88967209130303	-2.18374119165395	-0.77503189027831
C	2.00043399502291	-2.57243756377478	-1.79639479352737
H	2.57919229710865	-1.79734372537527	1.39683964251306
H	2.25863663621296	-2.76043025503712	-2.82784977993026
C	0.70547778431716	-2.68070420854151	-1.21755532692619
H	-0.19956456847146	-2.98263814678748	-1.72614234230344
C	0.81461779412826	-2.36657218969584	0.15777425278840
C	2.16415916704198	-2.05166236951929	0.43362734609875
H	3.95025784616695	-2.01366252294521	-0.89317089952127
C	2.64573826112505	0.44540495343980	-1.54170238845041
O	3.61806060516018	0.51555896534506	-2.19280575168242
N	-0.07437907132508	-0.12495415208137	-3.63195248726941
C	-1.17672262355986	0.52573270729550	-4.33954413590454
H	-1.94398038449211	-0.20356995309468	-4.59638865543802
H	-0.79304947727042	0.97124766271692	-5.25496343710930
H	-1.61802131100464	1.31021597201362	-3.73290525006497
C	-2.03369222550289	-0.12909221197483	-1.43516244879591
N	-2.99578537493706	-0.74645235742856	-1.57421838640516
H	0.00420921141353	-2.33708899641583	0.86699255724750
C	0.10157507738682	0.49450112317605	-0.17785398815718
C	-0.80121138779564	0.65804568258598	-1.41341936565532
C	-0.55829320689493	0.54583811161868	1.13569244116211
C	-0.05824397491381	0.07535938570650	2.38505755334400
H	-2.35505870749591	1.81428658742219	0.71624940543322
H	0.80061041856243	-0.56548960021060	2.51650545101441
C	-0.84697581958130	0.61274884297548	3.43393049001712
H	-0.69880926658907	0.44398486492087	4.49138594476410
C	-1.88567232604755	1.37582604696627	2.84657561157316
H	-2.66736226036643	1.90387112896973	3.37455374551814
C	-1.72456826664518	1.31226384484995	1.43826589195450
Fe	-2.00875696582648	-0.57101421068892	2.24243234120541
H	-4.57801845130893	-0.59968160312106	3.41524708024509
C	-3.84843437190958	-1.21763662501697	2.91106364751510
C	-2.81263731560801	-1.95955456193410	3.53469709834884
H	-4.38838287138988	-0.97680554303320	0.75994330315725
H	-2.61484622283971	-2.00844012758574	4.59606733304886
C	-2.07820652272847	-2.62131818351197	2.51917401195059
H	-1.22586641876999	-3.26758251597805	2.67511324039976
C	-2.65571353595652	-2.28401256103423	1.26884946694751
H	-2.32700620275352	-2.62949312087749	0.30040430883753
C	-3.74769647340057	-1.41279861178778	1.51155579949429
H	-1.10798635809686	1.67633658750840	-1.68879697156488
C	0.75610851338002	-0.95772233979722	-4.45021468236009
C	2.34876432414912	-2.61243622517350	-6.01821542998008
C	1.98725036126508	-0.50516411146326	-4.90173099448499
C	0.31180818525257	-2.21953816707852	-4.79896113281830
C	1.10115649253328	-3.05275900200461	-5.58005917526959
C	2.78245276680796	-1.32911462319305	-5.67445748749474
H	2.33145783155676	0.48672904969553	-4.64206902952169
H	-0.65041658487039	-2.57336648048163	-4.44939973455040
H	0.72845831238909	-4.03782153529199	-5.82510819295395
H	3.74882609662668	-0.98390463512459	-6.01931921673709
O	3.18917780578234	-3.34317141834825	-6.76864339149487
C	2.79942143736135	-4.64524512937031	-7.15327864103194
H	2.64541978512429	-5.29823935397257	-6.29010479950607
H	3.61323969379203	-5.04593745916020	-7.75242354978978
H	1.88886299769174	-4.63758866361012	-7.75820401213311
C	2.52318199479844	1.11974803464198	1.09263516267845
O	3.12457585986100	0.87114205025721	2.03269296027091
H	3.20111948436777	3.14921188309165	-2.37690212748805
C	2.44853132819148	3.26046336950375	-1.61085189077835
C	2.69551211151363	3.54133239627117	-0.25683587611489
H	0.55466234602940	2.94575493413993	-2.73844338137731
H	3.66493664256964	3.70678817520710	0.19122897556884
C	1.43484272556098	3.59816473452013	0.41481091984029
H	1.27646216021252	3.81875451904196	1.46054744734244
C	0.43016794236304	3.35040288488903	-0.53952380713229
H	-0.63062893252889	3.33215644667409	-0.33485899674472
C	1.05049332038240	3.12861647994965	-1.79618691879839

[1d]⁺ + CN⁻ (C2-CN, is4)

Fe	1.85118843445964	1.42686183088425	-0.04783407775932
Fe	1.38486865303260	-0.95360192846503	-0.59227369098771
C	0.05666671210582	-0.45663915357649	-1.84635704877715
C	3.01023274917378	-2.28845351663472	-0.14916575173385
C	2.21740189724527	-2.80614858099913	-1.20178202196903
H	2.52697604939273	-1.79767286147582	1.96045532889882
H	2.56231922344522	-3.04809385870261	-2.19597454595533
C	0.90502601660025	-2.98842154104940	-0.69668857841744
H	0.06081976656367	-3.37885127693178	-1.24830483368837
C	0.89326199395358	-2.58506389093861	0.65807623019555
C	2.19930963884250	-2.15202576909757	0.99579017664606
H	4.05945764796845	-2.03637371478119	-0.21231385633387
C	2.56124359654111	0.15776839679321	-1.37877367107772
O	3.41198011060076	0.25056367623686	-2.18274567366415
H	4.10306341723133	3.12572401286121	-0.54457713702983
C	3.51351705184215	2.68865638604392	0.24812896073927
C	3.75813451851527	1.45887875286469	0.89193316940357
H	1.90433492896969	4.20966516357133	0.58893671244632
H	4.56257133281183	0.77379073534516	0.66531011344190
C	2.76103026463717	1.26386305888607	1.87885062505844
H	2.68721032353718	0.42181696787392	2.54758052509131
C	1.89594398312934	2.38121488134147	1.85284058556588
H	1.03133713851613	2.53459747150776	2.48097668666263
C	2.34839290281397	3.25748706247031	0.84449282510700
N	-0.26226255237997	-0.63656313348825	-3.09285644904727
C	0.57700750219686	-1.40223231028819	-4.00613515974776
H	0.72702727446053	-0.83825534502528	-4.92487811656333
H	0.09142317114039	-2.34637886094511	-4.25056886975062
H	1.53858837419505	-1.59447419941551	-3.54568009991331
H	0.03863053518156	-2.60107528830763	1.31455068125442
C	1.25788054182420	2.29451933540427	-1.44681827223189
O	1.00231439019832	2.93356757083707	-2.36033412460531
C	0.22217274583990	0.37839435162245	0.24222022444143
C	-0.81778735424398	0.29258430494371	-0.88637976300184
C	-0.40463150883936	0.45092025364822	1.58024108087809
C	-0.05170094642210	-0.21934059263510	2.78446228892320
H	-1.96904698488968	2.02450898849574	1.25176696266535
H	0.71043271691653	-0.97497419871720	2.89114653980499
C	-0.85445081606378	0.26788067970837	3.84699495730556
H	-0.81280375205401	-0.06030727855374	4.87604569969290
C	-1.72932532341690	1.24447051486176	3.31491540901655
H	-2.47585620064001	1.80230224854614	3.86297412970653
C	-1.46659557633809	1.34589871471121	1.92586440843709
Fe	-2.05405819688215	-0.55702490579713	2.39872376524354
H	-4.80845677847981	-0.22375458656089	2.91957066824048
C	-4.07313319367143	-0.92895988827487	2.55945954863812
C	-3.34104661029411	-1.84881998894992	3.35286488412527
H	-4.03027966533638	-0.52596349153413	0.36436888256321
H	-3.42245867061382	-1.96999750102283	4.42363872180025
C	-2.47823489246376	-2.57743246372528	2.49618425873917
H	-1.79018726314116	-3.35408857363752	2.79891651818651
C	-2.67697868039346	-2.10712544036209	1.17244440568832
H	-2.17384225524918	-2.47023948525344	0.28696002416451
C	-3.66043313712043	-1.08608989346529	1.21222751227643
H	-1.60932642542973	-0.40896945794628	-0.58417551619003
C	-1.53007408624827	1.50587746327182	-1.28976774890933
N	-2.09908435457417	2.48047059947571	-1.52203362704166
C	-1.49172903890613	-0.15087861843745	-3.64799760998609
C	-3.88249411181340	0.83996174238271	-4.66447904671894
C	-2.69838627438247	-0.72192744197658	-3.26323030853100
C	-1.47895042929546	0.89231438504856	-4.55611488862869
C	-2.66675896553906	1.39063619881420	-5.06881555189338
C	-3.88668070297642	-0.22639749498761	-3.76154270458535
H	-2.71271970674491	-1.55353511509001	-2.56903542792570
H	-0.54060144162904	1.34207405916226	-4.85593011957355
H	-2.62356962778670	2.21463397602159	-5.76725671441067
H	-4.82917454317742	-0.66324680659542	-3.45722475657157
O	-5.08306636949411	1.26209296171012	-5.08827702565061
C	-5.14184403097147	2.31540132298498	-6.02888629831010
H	-4.70829882267500	3.23903438577394	-5.63685084544674
H	-6.19556375959412	2.48449692222707	-6.23554911167562
H	-4.63686155371128	2.05588807731303	-6.96306146674441

[1d]⁺ + CN⁻ (C2-CN, is5)

Fe	1.87038382770346	1.49264898743283	0.01493054405735
Fe	1.39866049658679	-0.84970232762317	-0.68478012647622
C	0.06213729207080	-0.30229720023892	-1.90588246072888
C	3.00253663573509	-2.24513813804600	-0.38900411689153
C	2.14965811861086	-2.67980494429900	-1.42915340444743
H	2.63298921034862	-1.85172658250705	1.76751956878213
H	2.43164266338844	-2.85359256895789	-2.45695896683078
C	0.85792751784517	-2.85862616105133	-0.86924191468678
H	-0.02249445192529	-3.20200186837983	-1.39433834397290
C	0.921711125424955	-2.53421373126007	0.50517521617567
C	2.25039007684400	-2.14808716733147	0.80275032041296
H	4.05442066768644	-2.01747271837982	-0.48855172509499
C	2.62927134779740	0.28311230499601	-1.34661936979804
O	3.54000039194152	0.41416600606614	-2.07453639916969
H	4.11246897380968	3.23240876589053	-0.35812669830095
C	3.51605766917798	2.75038324484076	0.40276347878088
C	3.76424111138664	1.49241648024686	0.98703517955296
H	1.88689829545835	4.23723208182767	0.79612715748046
H	4.57942196804425	0.82803777337544	0.73865221757386
C	2.75537608280179	1.23794114790370	1.94757171963395
H	2.68633897953407	0.36416839137534	2.57556679258414
C	1.87990236145591	2.34749917087667	1.96597904121302
H	1.00412719385052	2.45887742220975	2.58747395788667
C	2.33642422202598	3.27745848175769	1.00970754519748
N	-0.30762126352526	-0.51775850612638	-3.13327826032455
C	-1.58774831115934	-0.09524353867883	-3.70646860035805
H	-1.85896357734719	-0.77957333008547	-4.50566246087924
H	-1.51263326470642	0.91027320997517	-4.11865580513547
H	-2.37364232129128	-0.12365302969058	-2.95610990679522
H	0.09632176581143	-2.56572389265530	1.19742389164126
C	1.34040980537139	2.40892391289197	-1.37853771261780
O	1.13184253724157	3.06398391492479	-2.29273097414649
C	0.23271573264493	0.43572965186595	0.21840873964397
C	-0.80474064940312	0.42233893023217	-0.91719743092100
C	-0.39838167105719	0.43901098991241	1.55543533143128
C	-0.03086761335541	-0.27051963062286	2.73235147543210
H	-1.98357113836396	2.00257665844858	1.28928719461480
H	0.74326550681636	-1.01826102838534	2.80662651256522
C	-0.83084145653537	0.17148757128045	3.81680252480978
H	-0.77868721502819	-0.19158015945846	4.83360393089781
C	-1.72141899669279	1.15491505476781	3.32447433195499
H	-2.47038371534445	1.68428677073768	3.89691505577832
C	-1.47003177142853	1.30692947145765	1.93767531823866
Fe	-2.03026303994150	-0.61777470250282	2.34960435739112
H	-4.78056257085079	-0.35661964884117	2.93441283448760
C	-4.03964035154145	-1.03183714602322	2.53075185455927
C	-3.27758725291416	-1.97193781607180	3.27039806203009
H	-4.04434206277165	-0.53394125165116	0.35540058382867
H	-3.33663071451681	-2.14049713573310	4.33625728869249
C	-2.41869407179717	-2.64753589769660	2.36759049044521
H	-1.71115717269185	-3.42363075878273	2.62311506914172
C	-2.64891221853306	-2.12372698075156	1.06929326709816
H	-2.15563603682941	-2.43837751272105	0.16014311542504
C	-3.64881541492113	-1.12311532842431	1.17099269737626
H	-1.62549647554622	-0.26495006842732	-0.65623595257782
C	-1.45245351653913	1.67913944436803	-1.28553115235298
N	-1.96636710914388	2.67954912690224	-1.53566242511269
C	0.58623090398942	-1.18831566000882	-4.02832797222381
C	2.35480155332554	-2.48272156985153	-5.73996236009801
C	1.66248935231971	-0.49658211638829	-4.56512952683124
C	0.37438717285673	-2.51100743908464	-4.37121820005729
C	1.25513478145636	-3.16578647154978	-5.22126089245208
C	2.54475252151305	-1.13852544392884	-5.41098089518137
H	1.81464914605725	0.54430110944063	-4.31323998855463
H	-0.47119180087581	-3.05151731639766	-3.96370814980361
H	1.06993225526590	-4.20407483067500	-5.45877329421220
H	3.39082565069471	-0.60278349975953	-5.82196423109809
O	3.26961073978600	-3.02777261038338	-6.55842390172986
C	3.15352065531372	-4.39745410066389	-6.88561353034211
H	3.19472469854312	-5.03315083750212	-5.99714815851060
H	3.99879604947440	-4.63477357561556	-7.52649888245638
H	2.22934203974286	-4.61112683279118	-7.42905444993669

[1d]⁺ + CN⁻ (C2-CN, is6)

Fe	1.60227713759290	1.61960893712666	-0.34473353359150
Fe	1.32372963494405	-0.80785494110662	-0.88876507424858
C	-0.04360910715296	-0.39069575375461	-2.11805875920659
C	3.02120065631452	-2.12775411943241	-0.58769300696604
C	2.17730234529900	-2.61440461978822	-1.60996682150141
H	2.66614914775402	-1.74423592477167	1.57355705077698
H	2.45825211308770	-2.79310824071483	-2.63710610601975
C	4.06072083514233	-2.84833396451379	-1.03084896586928
H	0.03444097322096	-3.24214578115008	-1.54141839776820
C	0.96851404941913	-2.50053973307999	0.33728941486437
C	2.28143789220881	-2.04995729096056	0.61291773163369
H	4.06072083514233	-1.85672400158572	-0.70336490665192
C	2.54457017590500	0.37942912937272	-1.52921211557566
O	3.48450346336465	0.46771219440701	-2.22131495332737
N	-0.40525519937125	-0.68663349132801	-3.33195462418681
C	-1.72219170120619	-0.40485185922205	-3.91148938388584
H	-1.92393669011947	-1.13118145898471	-4.69348543036433
H	-1.74684434200750	0.59215482177359	-4.34878817442191
H	-2.50247581586593	-0.49395763420938	-3.16043401802498
H	0.15745693600633	-2.56338782349176	1.04496751728112
C	0.09193924244267	0.40089918166239	-0.00733102775143
C	-0.95748787736356	0.27360158247500	-1.12848064898709
C	-0.48659187796325	0.43831450117545	1.34971044105305
C	-0.03210819660087	-0.20520053446036	2.53628067147536
H	-2.17380973451810	1.89275683403151	1.09232618949260
H	0.78084299515658	-0.91124256497692	2.60434479564313
C	-0.81102239655342	0.23619059027720	3.63630280583205
H	-0.69541639206468	-0.08210885092078	4.66289660821391
C	-1.77291738768088	1.15118010930618	3.14658730174941
H	-2.52580532397575	1.66180824616810	3.73058242529079
C	-1.58628031508201	1.26300844038334	1.74541237327244
Fe	-2.02245109859872	-0.67025805212185	2.25088529801072
H	-4.75929991801735	-0.51718207858779	2.92678005677659
C	-4.00215836366292	-1.16971406015325	2.51601892143526
C	-3.17173196098016	-2.05061878298001	3.25520283114551
H	-4.10034072597839	-0.73416860957650	0.32936375811457
H	-3.18801113859334	-2.19070688362112	4.32665038034192
C	-2.31307563098658	-2.71302069900392	2.34200764635865
H	-1.56356419074686	-3.44991707857801	2.59431645518450
C	-2.61323278747548	-2.24095529804983	1.03801061668780
H	-2.13746559288977	-2.56159766276434	0.12170538864348
C	-3.65456568779945	-1.28425070903882	1.14613492220131
H	-1.68594548400426	-0.49993584798762	-0.83372887474757
C	-1.79194118944826	1.40235703752102	-1.54085319233693
N	-2.48733058195748	2.26882205055363	-1.84700400782314
C	0.52808966683826	-1.34166386733435	-4.19786169225545
C	2.37361169394684	-2.63108790120897	-5.83302132351598
C	1.61798279185111	-0.64389071787601	-4.69716251435807
C	0.34447914193488	-2.66971167486369	-4.53917032668104
C	1.26133161363833	-3.32112121551622	-5.35224178981892
C	2.53838856951264	-1.28329918179891	-5.50422345050631
H	1.75215474682765	0.39959404180219	-4.44678471277290
H	-0.50851595549903	-3.21762331258790	-4.15748357230098
H	1.09465316547801	-4.36256946516995	-5.58976274586670
H	3.39449839862604	-0.74233031675660	-5.88673025279966
O	3.32291352208352	-3.17350253269766	-6.61301220337446
C	3.22221358868544	-4.54276119772511	-6.94784683928730
H	3.23307812724266	-5.18102856112693	-6.06032990386463
H	4.09066427046542	-4.77639387737373	-7.55839888275239
H	2.31898552007381	-4.75751667712995	-7.52519266036134
C	2.45715244006112	1.15809275808792	1.11775877663427
O	3.05666634818758	0.95673457739509	2.06969060650727
H	3.65135296695009	3.64513712382642	-0.16274092674183
C	2.63160869100353	3.47575612812284	-0.47717520254840
C	1.46484360121167	3.59668330723391	0.33747325366068
H	2.85850284458889	2.97516340026739	-2.62208474141947
H	1.44131565425192	3.88119709312378	1.37997984439126
C	0.34424867618608	3.31605507329019	-0.46654225755955
H	-0.68026012681457	3.35010460973842	-0.13274671533889
C	0.80125290257328	3.01700618709826	-1.77813316195075
H	0.19366921637641	2.80218309744769	-2.64340396228294
C	2.21003948685593	3.13538979641371	-1.77413622105830

[1e]⁺ + CN⁻ (C1-CN, is1)

Fe	1.72836943582655	1.39675682354240	-0.00221010238157
Fe	1.30962447005687	-1.03190338614608	-0.51486041958523
C	-0.13004730119260	-0.68127362276257	-1.96126195833642
C	3.06644899594608	-2.18968895398307	-0.55683154818031
C	1.99912493276946	-2.89282255534805	-1.15279184074061
H	3.35324820354694	-1.43869705118575	1.52407613449458
H	1.95424492961661	-3.23652643349666	-2.17583742838570
C	0.98999234059342	-3.05675075854464	-0.16959676746304
H	0.04711069979344	-3.56338828838135	-0.30749561613249
C	1.44971441726281	-2.47232537337954	1.03485779935157
C	2.72588046094749	-1.93080369886987	0.79818174016033
H	3.99278400716765	-1.91428071976642	-1.03919553926905
C	2.31452080923693	0.32524639885184	-1.44505001611045
O	3.07140108496051	0.38168579185101	-2.32536686519755
H	4.08673284729159	2.88625461132658	-0.69527963389445
C	3.50596870879703	2.53722914445476	0.14543653934793
C	3.67538552080694	1.31549881233505	0.83749450150206
H	2.06725690264105	4.20257906746194	0.48873647021118
H	4.41508223083266	0.56128891066945	0.60872552837115
C	2.72094803647335	1.25213004065289	1.87932315649575
H	2.61119352571196	0.44920622238936	2.58927729519716
C	1.94848766870607	2.43254663950391	1.83603786362379
H	1.13096215165826	2.68851186499383	2.49356422329159
C	2.43753202823638	3.22609757228125	0.76917540162134
N	0.02869488752357	0.25406498447138	-3.04789364203746
C	0.66633973338832	-0.35888356884321	-4.21145327780600
H	1.05908866808519	0.39225693963757	-4.89002995802748
H	-0.02878295724304	-0.98734354549183	-4.77725376977712
H	1.50116634530461	-0.97849894184912	-3.89210779051900
C	-0.61654753991317	-1.96405890565703	-2.42370420874113
N	-0.93933149771777	-2.99727849643716	-2.82720304136387
H	0.90140633150332	-2.43576680521663	1.96464273520255
C	0.59894129285812	2.39838345929745	-0.91190271495509
O	-0.16025674163895	3.16548924567801	-1.27378505653323
C	0.11889901884815	0.35788791404210	0.32928387061864
C	-0.59284190470952	-0.37310308442547	-0.62494303639984
C	-0.53747119806079	0.53656665818557	1.63751643783735
C	-0.12654403396797	0.13835542230788	2.93787398741124
H	-2.24536216900256	1.81527584779828	0.99186407089105
H	0.70984551032327	-0.50205670851104	3.17295485148005
C	-1.00131287788742	0.72370275555989	3.88809845140058
H	-0.94954465099703	0.59528137527247	4.96001075616664
C	-1.96960077839738	1.47997852914464	3.18351992464501
H	-2.78580531663206	2.03713080573183	3.62093374980756
C	-1.69297737136932	1.35480742387017	1.79952710741145
Fe	-2.06103122096268	-0.49190091056383	2.62194718258163
H	-4.87805510377344	-0.39485347214883	2.81299682291480
C	-4.03685328996941	-1.06674659750488	2.71973133689710
C	-3.30733672888421	-1.64223337830117	3.79114521705073
H	-3.78820658214127	-1.25483438583931	0.51024176110754
H	-3.49432523450512	-1.48285151585860	4.84357773514132
C	-2.28006257328113	-2.44880368681790	3.24026048419880
H	-1.55108429157036	-3.01819620031278	3.79897403582060
C	-2.37720234449112	-2.37580165963132	1.82831979968427
H	-1.74192543318564	-2.88956001421471	1.12206101354729
C	-3.46140811832917	-1.51959319378324	1.50618026459459
H	-1.42467018669785	-0.96734796365563	-0.25952964667325
C	-0.96587818682897	1.20385511702598	-3.39509065437021
C	-2.80408690532875	3.22946181936390	-4.13401531251748
C	-2.34912581245015	1.06429014382749	-3.20970375472412
C	-0.52900710274254	2.41033036792922	-3.99141424338663
C	-1.44808853408329	3.38204786865077	-4.36303720308353
C	-3.25245798035787	2.06517004707342	-3.54608432474049
H	-1.08130716409325	4.29772254397167	-4.81094316231549
H	-4.30772195668594	1.90997312091744	-3.36652038588646
H	-3.50481826415348	4.00677537685237	-4.40719230074390
Cl	-3.08245727836416	-0.38903664360852	-2.602357157330038
C	0.92307642949818	2.72619906954067	-4.21332664208734
H	1.57932499166157	2.20603097230826	-3.52110704701835
H	1.09098132690319	3.79689520075591	-4.10398280323554
H	1.24240068683184	2.45879961100755	-5.22309638015893

[1e]⁺ + CN⁻ (C1-CN, is2)

Fe	1.68727102146724	1.41760121232142	-0.01250799423280
Fe	1.27561390492860	-1.02473555216512	-0.50738041467280
C	-0.18014536336151	-0.68901885206107	-1.94428777149021
C	3.04677642020362	-2.16116008392968	-0.57703320119415
C	1.97885892458484	-2.87922086872140	-1.15273145379863
H	3.35866899987126	-1.40024843286486	1.49695287294510
H	1.92124471520060	-3.22728649083056	-2.17380062930305
C	0.98793329056175	-3.05202478567253	-0.15194977912531
H	0.05132501805135	-3.57469896002138	-0.27194803515392
C	1.45977491507403	-2.45759005778992	1.04247137535263
C	2.72538638076326	-1.90164151965015	0.78258517090994
H	3.96114349465720	-1.87538621803135	-1.07586781712292
C	2.26246535805909	0.36601342033037	-1.46406475735071
O	3.00856417092203	0.40577502577527	-2.35036646747645
H	4.02837908700310	2.91407092405979	-0.74751231590915
C	3.46108577563231	2.56799718253956	0.10353495815990
C	3.64618539752764	1.35138260014947	0.80219989098090
H	2.01917006692481	4.22757625192851	0.45246379100288
H	4.38703046754164	0.59979727643980	0.56877897908874
C	2.70621986889055	1.29027624606398	1.85630806743836
H	2.60893860963053	0.49031680730447	2.57116130276536
C	1.92584450671343	2.46579217107445	1.81427978211426
H	1.11521003220739	2.72186579890278	2.48028841604755
C	2.39849067515613	3.25548286080085	0.73619733147111
N	0.00739065737999	0.21795912285202	-3.04645145723194
C	0.62698292131223	-0.42895632285215	-4.19995176557245
H	1.01390875721508	0.30598551500393	-4.89960947798657
H	-0.07727561504453	-1.06977626953684	-4.74114272929885
H	1.46388653864153	-1.04438719244796	-3.87618701698232
C	-0.68389877302696	-1.97547878258742	-2.37288037826029
N	-1.04180128053087	-3.01050361589662	-2.74193087210323
H	0.92635410540667	-2.42323801664445	1.98089307258409
C	0.50849113954219	2.40653153542770	-0.87551245896908
O	-0.28665889676357	3.15614985166451	-1.19339359763320
C	0.09387909284670	0.36068456858633	0.34649728435409
C	-0.62703510592363	-0.36709111319864	-0.60406293137960
C	-0.54958222426088	0.53287821421056	1.66208686744599
C	-0.10993411012514	0.14299764021489	2.95572989668287
H	-2.29151983210428	1.78009300345579	1.04550686542789
H	0.74205377902837	-0.48169049900912	3.17634757603796
C	-0.97978823467309	0.71115233429758	3.92032398872380
H	-0.90793955936055	0.58344947425296	4.99114572406229
C	-1.97417216047533	1.44842043370721	3.23195805517619
H	-2.79342985489090	1.98965721776198	3.68332594733160
C	-1.71780554753593	1.32904289169308	1.84351472023410
Fe	-2.03620514363969	-0.52463805777774	2.67137021990026
H	-4.84717756899766	-0.49277933375413	2.95301062069660
C	-3.99416127662155	-1.14456753322343	2.82940886487453
C	-3.21749423419349	-1.70795807577296	3.87371485034879
H	-3.81856496283869	-1.32327869044254	0.61233319043856
H	-3.37320667506963	-1.55711732321498	4.93247832208297
C	-2.19020694993010	-2.48790111375967	3.28559722397965
H	-1.42954394787856	-3.04166620348273	3.81707990663412
C	-2.33493260851621	-2.41152587901270	1.87792345875185
H	-1.71228144088308	-2.90769001940349	1.14835937963108
C	-3.44871512945428	-1.57966913118826	1.59554605361672
H	-1.45600043070316	-0.96076781188635	-0.22712646481131
C	-0.95068737670149	1.19969343528828	-3.40358078244137
C	-2.64510544903198	3.31476755746933	-4.20680206482989
C	-2.35060878581217	1.06840573764636	-3.31384354575712
C	-0.45894259179703	2.40925692524801	-3.92688099140206
C	-1.27527569684158	3.44565930347900	-4.33941502068656
C	-3.16038384073238	2.14018791491812	-3.69247273122683
H	-0.83876649718930	4.35325826445031	-4.73338513278157
H	-4.23410400056477	2.02768835228631	-3.60674858854167
H	-3.30215110994965	4.12005733626115	-4.50638729641901
C	-3.05893300730362	-0.18301777469535	-2.87780772076678
H	-2.92617237254170	-0.40336538620004	-1.81885891326160
H	-2.74051835003791	-1.05589995318159	-3.44336524387434
H	-4.12966024085176	-0.07096205689616	-3.04190299887276
Cl	1.25125015321348	2.69543856993721	-4.01339520937222

[1e]⁺ + CN⁻ (C1-CN, is3)

Fe	1.63276070436814	1.80844337349491	0.46958700979991
Fe	1.22010065104322	-0.47020875850417	-0.58892607962524
C	-0.22377240387760	0.21514043776655	-1.87943519774884
C	3.02312092306788	-1.55442328835351	-0.74878289682860
C	2.05612094810298	-2.09198779801226	-1.62138768173663
H	3.05490837610795	-1.34694228245073	1.47265950545062
H	2.13713918409528	-2.15911067520647	-2.69473002645667
C	0.95655600395170	-2.51899769647800	-0.83317023291112
H	0.05288730042166	-2.98193714093949	-1.20114509912029
C	1.26358470161385	-2.26239386134326	0.52335610812954
C	2.53369003252070	-1.65664407344997	0.58048840294211
H	3.98126129918100	-1.14756595670203	-1.03786738062624
C	2.26186519373495	1.09419930508291	-1.14844827746871
O	3.04521636044389	1.31062436134296	-1.97472911746353
H	3.90815496856534	3.49959983338135	0.01676228048735
C	3.36735805969857	2.97619639729744	0.79099817962361
C	3.61155476848960	1.65630867527821	1.24624641334328
H	1.86662239457344	4.47865760476976	1.45809422299435
H	4.37503415558287	0.98997518782314	0.86999871403989
C	2.69540704627761	1.36180773273513	2.27892527375837
H	2.65255364686627	0.44458391761798	2.84318002611453
C	1.86613035016896	2.48887608691551	2.46294555015462
H	1.06175715829765	2.58349949699856	3.17764646434801
C	2.28964120425735	3.48775325726754	1.55010444543801
N	-0.14313815560599	1.42137645164099	-2.68514871361812
C	-1.47494084753060	1.91560995818064	-3.03490192020637
H	-2.01300786978622	1.23126469673491	-3.70040477803300
H	-1.41515921637421	2.87616845742505	-3.54095390740899
H	-2.06735583607363	2.04778215378620	-2.12996896863453
C	-1.04811356974401	-0.82715939807269	-2.48113354137456
N	-1.79138688194456	-1.63149419881460	-2.84799750359077
H	0.60946423355459	-2.45170309906665	1.36104301498524
C	0.33261472345438	2.83961646664758	-0.14247513499599
O	-0.56380895455210	3.53225988647540	-0.27090550788794
C	0.08091446680541	0.66576956648466	0.61261892374637
C	-0.66224100012461	0.22198345456349	-0.47629115273579
C	-0.51433509924314	0.48576343583759	1.94775062381300
C	-0.01409341702311	-0.21287828392316	3.07875630255520
H	-2.30249558294059	1.80108539606792	1.73695976669343
H	0.85876735384135	-0.84808737146544	3.09815171309347
C	-0.85118508079970	0.06534446809686	4.18830440764476
H	-0.72999155454023	-0.32970489028375	5.18695426641975
C	-1.88628984030979	0.92736645819081	3.74969135108491
H	-2.69491295393034	1.31244839584420	4.35436377969596
C	-1.68712245436142	1.17600000752292	2.36903231152835
Fe	-1.94081866135190	-0.83627924354449	2.70273057912564
H	-4.69694771132053	-1.00089983194299	3.28407858321260
C	-3.86324324170226	-1.55037169114122	2.87060428061395
C	-2.96869591256915	-2.37787669072354	3.59667741284385
H	-3.94199532649747	-1.02687922967468	0.70168761607713
H	-3.00073078821730	-2.56934547527379	4.65980273978400
C	-2.01686604321108	-2.90058544806603	2.68522819473958
H	-1.20154261775874	-3.56634745147974	2.93086285040873
C	-2.32689722121340	-2.39988846041534	1.39602685185039
H	-1.80009484314765	-2.63063545455852	0.48085331405791
C	-3.46521678951727	-1.56264096202713	1.51004959940024
H	-1.51189039716237	-0.41330115736526	-0.24009127324085
C	0.81119020117223	1.64608695225539	-3.72546042275875
C	2.69877815202072	2.26959175410957	-5.75916418457091
C	1.27551051827789	0.69714479890565	-4.64568448847168
C	1.31084677789732	2.96063451630357	-3.89356325814101
C	2.22170804532655	3.24561525305086	-4.90328586727731
C	2.22050031895840	0.98545341427588	-5.62409066247433
H	2.58196500928438	4.26212211510544	-5.00240644180176
H	2.55196430525510	0.20025823632464	-6.28980697898348
H	3.42362179718477	2.50653594250830	-6.52624252993835
C	0.96305894271964	4.10296453285637	-2.98438873701528
H	1.53094195708607	4.03841428308783	-2.05549504584876
H	-0.08927630466225	4.17045911544590	-2.72862725342612
H	1.24076933842601	5.04464550528780	-3.45571216727821
Cl	0.69127500439754	-0.93211447150947	-4.68904665029990

[1e]⁺ + CN⁻ (C1-CN, is4)

Fe	1.62631542475134	1.81156527742398	0.46103524783518
Fe	1.22772560388087	-0.47558286887127	-0.58923524073231
C	-0.22366403978882	0.20394416914813	-1.88225383885028
C	3.04120908368488	-1.54970183285523	-0.72260135029319
C	2.08789557055878	-2.09997079692350	-1.60244906762299
H	3.04716591308400	-1.33035019744847	1.49667813447818
H	2.19507996884640	-2.18916563891175	-2.67263419444453
C	0.98134718017028	-2.52987571739181	-0.82480398731708
H	0.08549543442447	-3.00282503713271	-1.19924352246853
C	1.27130674683244	-2.26151359318484	0.53290204351729
C	2.53676746521214	-1.64665286927630	0.60059903005983
H	4.00019209433360	-1.13935372476501	-1.00354894828841
C	2.27351629431615	1.09568586822338	-1.14504151513546
O	3.06618755127985	1.30028415374272	-1.96442561745932
H	3.89688316869835	3.50875589006702	0.00743098864629
C	3.35519722018450	2.98933999237137	0.78356055580058
C	3.60238442731575	1.67368858509383	1.25008129949069
H	1.84573397113573	4.49083430831884	1.43090925406156
H	4.37114344916008	1.00798575580169	0.88361246065335
C	2.68178780282225	1.38329391498705	2.27958967683394
H	2.63997286255783	0.47044788882521	2.85086951276429
C	1.84681660367217	2.50856152895222	2.45038625033012
H	1.03801155513204	2.60556537700795	3.15975209969809
C	2.27223515573411	3.50248013901286	1.53326030348894
N	-0.14672248334461	1.40566480401028	-2.68973633559777
C	-1.46749211416346	1.93774966351227	-3.01758761589901
H	-2.01336548461531	1.30294507956442	-3.72531714201325
H	-1.38754334985856	2.93102248988527	-3.45379561917288
H	-2.06208168893613	2.02095324173267	-2.10848098068826
C	-1.03518949059107	-0.84518021772628	-2.48300834902481
N	-1.74498972495828	-1.66472792107447	-2.88151156729727
H	0.60866563748390	-2.44851548069115	1.36447395663090
C	0.32291826198837	2.84540381549279	-0.15967650572412
O	-0.58082739959172	3.52980793103025	-0.26827959347199
C	0.08071662770342	0.66221742338981	0.60887185094867
C	-0.65853981566383	0.20732021798616	-0.47733663692658
C	-0.51571905247206	0.48593602946679	1.94394625987468
C	-0.01524812182668	-0.20176644080789	3.08163711055452
H	-2.30744341786547	1.79384834198007	1.71930166246832
H	0.85950446299761	-0.83415380226327	3.10805117050332
C	-0.85451306833640	0.08397285134134	4.18772621716734
H	-0.73336239879245	-0.30146921018204	5.19014326392354
C	-1.89162152346612	0.93895402430738	3.74014381230331
H	-2.70217023537620	1.32705460792634	4.34031441650199
C	-1.69120175777390	1.17613827914996	2.35774319791537
Fe	-1.93921019345217	-0.83441899027729	2.70963416075379
H	-4.69460199253270	-1.00599821657708	3.29478380992948
C	-3.85865736650597	-1.55545218039843	2.88584662842652
C	-2.95982377771134	-2.37184249206447	3.61906063689103
H	-3.94188281432225	-1.05357250267696	0.71215199767718
H	-2.99022634843621	-2.55306322337973	4.68404151003288
C	-2.00618403468984	-2.89878521737717	2.71194392004924
H	-1.18739292949837	-3.55795630236861	2.96376526928989
C	-2.31927645781001	-2.41180915235178	1.41813173144358
H	-1.79167796057865	-2.64886962321484	0.50490998322760
C	-3.46151786600619	-1.57883828581289	1.52522867094826
H	-1.50532791832395	-0.43211134668573	-0.24032560502510
C	0.81430320705124	1.61142646252708	-3.72540202797987
C	2.77566054077502	2.25464060660816	-5.67750344349551
C	1.22493828465030	0.66280192113168	-4.68508402250983
C	1.37966310242491	2.89349593436151	-3.85226721795893
C	2.33210065387956	3.22373968630123	-4.80036199134332
C	2.21417862711180	0.99539123540891	-5.61144771198579
H	2.72981759835660	4.22873445898110	-4.83596539094625
H	2.52551034296121	0.23997876272577	-6.32199066855781
H	3.53210202064481	2.48658233625316	-6.41509517890700
C	0.61956799554449	-0.70042623640278	-4.84358826378348
H	1.02716978578593	-1.18101061947025	-5.73199661417023
H	-0.45884902470618	-0.64964981030429	-4.97357325795462
H	0.82218471379567	-1.36141594538563	-4.00571920712045
Cl	0.92588644105203	4.18429244020323	-2.79028586495350

[1e]⁺ + CN⁻ (C1-CN, is5)

Fe	1.51837997829642	1.81177684636202	0.32159719667112
Fe	1.41417703469415	-0.54680095003571	-0.68708316865222
C	-0.00794629505502	-0.07798414049584	-2.08577043719797
C	3.11134210866134	-1.69066742261377	-1.23050688518465
C	1.94542435504449	-2.42656790329641	-1.50490195252132
H	3.94161385407472	-0.92789449052358	0.68618755934454
H	1.63115586371797	-2.77751563137172	-2.47428829242299
C	3.86575157061448	-2.59657879194221	-0.29898023256809
H	0.29537469599339	-3.11621344924262	-0.19028576299434
C	1.99079996312360	-2.00069802878341	0.74614961083295
C	3.14628841065036	-1.44410124638731	0.16939510313504
H	3.86575157061448	-1.40519058848244	-1.94752938172576
C	2.47455627347098	1.03159067342930	-1.13613016417173
O	3.32037917031837	1.29861249404103	-1.87558518351004
N	-0.24085886209705	1.06777021682166	-2.94240503395863
C	-1.65809840670129	1.18929675381516	-3.27743915260863
H	-1.81805977958705	1.89811600616654	-4.08266365101702
H	-2.23910859897025	1.51642297853583	-2.41248261109215
H	-2.07278191909298	0.23734753904123	-3.62274304273928
C	-0.48135640088891	-1.29333717259814	-2.72753825121122
N	-0.91057650669678	-2.25002073039886	-3.21267307690845
H	1.72555501648547	-1.98895100733035	1.79204933848509
C	0.02239967401824	0.56926909909784	0.35446514309175
C	-0.56698429178441	-0.05952484964505	-0.72573976750965
C	-0.70446645457531	0.50077325579915	1.63759530486544
C	-0.32629375520588	-0.03246540656794	2.89923947162697
H	-2.45948915453670	1.75492962560342	1.07324771178335
H	0.53068728825957	-0.65661280026980	3.10076168881484
C	-1.27890448055699	0.37297305275414	3.86824234720743
H	-1.26452683562732	0.11036942922779	4.91656401421271
C	-2.26106181657062	1.15726473760903	3.21569678093197
H	-3.12900823331945	1.60682178177846	3.67660545209237
C	-1.91802179523830	1.22149627247096	1.84236320231199
Fe	-2.21065337140857	-0.72513278885491	2.40746135634739
H	-5.03207037696175	-0.76521862548949	2.35235233881763
C	-4.15416896651238	-1.38971978741011	2.26826121128195
C	-3.48944646238100	-2.04102695208801	3.33853672440083
H	-3.71172231087943	-1.34109374483581	0.08163337705252
H	-3.77236533555436	-1.99888723369463	4.38077748389583
C	-2.38077573405586	-2.74439265860153	2.80424991819816
H	-1.67305748340840	-3.33717648778236	3.36583223055098
C	-2.36346468923335	-2.52978559310667	1.40360008458166
H	-1.64972107222635	-2.94396429876828	0.70784610373762
C	-3.45760307977297	-1.69131163085002	1.07189472048938
H	-1.36956129129833	-0.76290822185823	-0.50993860738083
C	0.66766730187361	1.66148169045509	-3.83092751122442
C	2.49487797853675	2.99963788796387	-5.54970513208440
C	1.70649075308732	0.99481555013435	-4.49894378503208
C	0.53775544747931	3.04623313116860	-4.11565617870847
C	1.44084152097909	3.67712429369171	-4.96318168017376
C	2.62081273702031	1.64595543297580	-5.31481455465402
H	1.31950837471069	4.73792760673771	-5.14668138062222
H	3.41371813666730	1.07674476616728	-5.78086925303191
C	2.36261410175606	1.05744677539345	1.68448069153721
O	2.92586634683433	0.68484348306102	2.60129136197372
H	3.47677001217764	3.85214895295503	-0.30609176610581
C	2.44899861429023	3.69505172294831	-0.01451448714304
C	1.95744756583689	3.64870039865682	1.30493907409803
H	1.39253457546144	3.57901675730206	-1.96514112770406
H	2.55180134265887	3.73554102953385	2.20423957415558
C	0.55984042766846	3.42915984744770	1.25910800971624
H	-0.09915288615139	3.33682263419776	2.10935450112161
C	0.17799082401245	3.39212658124034	-0.10894939319928
H	-0.82850834299382	3.26075179727194	-0.47589189069140
C	1.33606153777810	3.55714969797099	-0.88996786622237
H	3.20025282783582	3.51329035520533	-6.18865726436494
C	-0.55092183275385	3.91080180757730	-3.53596354897972
H	-0.93281892843955	3.53927276116353	-2.59042402329791
H	-1.40119501379919	3.98889724987118	-4.21664887385008
H	-0.18104647400059	4.92295454563243	-3.37478541635751
Cl	1.89718113892096	-0.72473788595192	-4.41876989854150

[1e]⁺ + CN⁻ (C1-CN, is6)

Fe	1.55624105681177	1.77774333107484	0.31921743650073
Fe	1.42135569356216	-0.58414866704703	-0.67685003099478
C	0.01025501418780	-0.08302980564389	-2.08990985176566
C	3.13085838319968	-1.75593358552868	-1.15596398045132
C	1.96498570773242	-2.46492982041024	-1.49620964595064
H	3.88387236309413	-1.03537367592123	0.80721569069175
H	1.69508927321944	-2.80209931045285	-2.48507687624869
C	1.19193869749829	-2.63203091502986	-0.32827387225203
H	0.24146587214069	-3.13974470450498	-0.27119115855136
C	1.90905341163040	-2.06292466443743	0.75885038967719
C	3.10196902479262	-1.52421923462459	0.24619113243966
H	3.93006948179566	-1.48317139421695	-1.82889680981490
C	2.52187373720678	0.99494100836218	-1.11034348591682
O	3.37811914912382	1.22644762106690	-1.84973275447498
N	-0.24524941515677	1.06102305492624	-2.94494798340691
C	-1.67111491465677	1.17205830377134	-3.25506133894223
H	-1.84508323543803	1.79993454851960	-4.12304064760332
H	-2.23568646115827	1.57994409372041	-2.41469699409345
H	-2.09445298150982	0.19343805687979	-3.49927613993195
C	-0.44814229165252	-1.30317771834065	-2.73201137494661
N	-0.84088663670909	-2.26782252315181	-3.23311060747068
H	1.59484830895975	-2.05645066835737	1.79119569544344
C	0.04347342167841	0.55328668138275	0.35251115283255
C	-0.54893262967227	-0.07077760293836	-0.72870863970212
C	-0.69542040717978	0.50565322238241	1.62923418338600
C	-0.32842609519596	0.00546633055329	2.90759910461245
H	-2.44634427227595	1.74194271197849	1.01567409374458
H	0.52904677382199	-0.60892937280706	3.13557583684074
C	-1.29283357141643	0.43088768779956	3.85608015882859
H	-1.28882631193844	0.19388372376728	4.91053530243953
C	-2.27043233822962	1.19598421574437	3.17455693766963
H	-3.14469512239948	1.65343184373836	3.61529837700008
C	-1.91350924737512	1.22780672660389	1.80382563419852
Fe	-2.20559769887891	-0.70454304499158	2.41139405259472
H	-5.02652102009169	-0.74952856104485	2.34476125247846
C	-4.14744294885576	-1.37438726002296	2.27713694401176
C	-3.48662462845205	-2.00285044986020	3.36335318733402
H	-3.69487500894280	-1.36881795764679	0.09210035376780
H	-3.77440881570751	-1.94006521718454	4.40322952192013
C	-2.37425451712029	-2.71473144768253	2.84848737137193
H	-1.66842732735281	-3.29484866630072	3.42545873486530
C	-2.35024288912537	-2.52788498115473	1.44380777717979
H	-1.63201582776216	-2.95339895573931	0.75976826726576
C	-3.44479737264778	-1.69868752036776	1.09033700648946
H	-1.36294013108999	-0.76244473856075	-0.51622578480892
C	0.65258953033842	1.68050664970508	-3.82599386571375
C	2.40514325745800	3.11105984386037	-5.55205897491781
C	1.68334191808506	1.02151742676137	-4.53399908853364
C	0.51693924467114	3.06176485647963	-4.08777805744368
C	1.35998836493333	3.76621313576017	-4.93241088185723
C	2.54730664417346	1.75142356322937	-5.34617333370046
H	1.19987530293428	4.82475803914293	-5.08540025899111
H	3.33739917029794	1.21879278982447	-5.86088726497072
C	2.38842277494456	1.02943359173473	1.69408595058793
O	2.94378012518154	0.66336655799599	2.61801538539564
H	3.56095063067880	3.80050385183593	-0.18442283463165
C	2.51656126607990	3.64895523284989	0.04418318905902
C	1.94360423157019	3.60744846182380	1.33282546009837
H	1.57894206660838	3.54988755282028	-1.96610291917523
H	2.48215806135931	3.69007084434369	2.26694876904697
C	0.55180362163381	3.40014176382834	1.20024546464916
H	-0.15653866015518	3.30825998476962	2.00966017686475
C	0.25154261060572	3.36432183941905	-0.18901253209181
H	-0.72954850879691	3.24147546551570	-0.61912972768340
C	1.45672727904481	3.52507281115042	-0.89639983973290
H	3.08318483555798	3.64940461549902	-6.20009878081191
C	1.86932029480569	-0.46603600363406	-4.52499007759122
H	2.65872304096531	-0.74396852930648	-5.22166381648679
H	0.96516214684301	-0.98542081098104	-4.83799671320931
H	2.14835603247436	-0.84714925330166	-3.54851131440140
Cl	-0.73351853475728	4.02063102057135	-3.34069673201496

[1e]⁺ + CN⁻ (C2-CN, is1)

Fe	1.84120495816672	1.25946597114795	0.02451133272150
Fe	1.58507399843703	-1.02611997134912	-0.83738799855976
C	0.15779670458489	-0.63947985228056	-1.97377075541806
C	3.41584646223633	-2.05575687296990	-0.36904032183447
C	2.92260579549398	-2.49564360724424	-1.62457954889234
H	2.51576665648064	-2.10614257895933	1.66727150615681
H	3.44756918500490	-2.44094320052378	-2.56724856575019
C	1.64328471047578	-3.05241510607935	-1.40695902541362
H	0.99889763351294	-3.48073509260464	-2.16229184074764
C	1.34020882877927	-2.94949979011098	-0.02843719611229
C	2.44493203952954	-2.33248676865545	0.61345200806540
H	4.37254806229818	-1.58073017190063	-0.20849304849301
C	2.36631120018271	0.42809132082634	-1.63223022979424
O	2.95641999237762	0.76544145741067	-2.59034695120675
H	3.16069919159832	3.77229322948791	-0.15630935126672
C	3.11295322178336	2.87661350563931	0.44643135807753
C	3.90706787906040	1.72967066725167	0.29043963153286
H	1.52719153807168	3.36350610397233	1.94790325733597
H	4.67089622259494	1.58182666505325	-0.45868592887641
C	3.54089840374966	0.79959668993408	1.30141757678776
H	4.00056199854411	-0.15901560875692	1.47390919150081
C	2.52974483406016	1.37530249066570	2.08430191946342
H	2.04333677262064	0.90941263176619	2.92624939536386
C	2.23383741306258	2.64970742438497	1.54985328232693
N	-0.16967944144563	-0.72277934899261	-3.23114139488247
C	0.77139782805843	-1.15743400476715	-4.26005266444193
H	0.89360780953967	-0.36236303434501	-4.99476704281935
H	0.39130072071963	-2.04477944675669	-4.76284459818901
H	1.73091689454071	-1.38324312904632	-3.81193436096079
C	-1.65193555773063	-1.28495640203982	-0.64106911816656
N	-2.28286728430859	-2.23683609166849	-0.49856404877141
H	0.44077278773230	-3.31153275932121	0.44460836567147
C	0.65592783869494	2.29812258681780	-0.70091793530809
O	-0.12536577776654	3.06422985666924	-1.04186754785083
C	0.28753885089551	0.00344369588203	0.21581185788670
C	-0.78197467693492	-0.14234709982438	-0.90276417173560
C	-0.24805418618588	-0.08487169512503	1.60689879907630
C	-0.55306033015578	-1.24651353037440	2.37220518707313
H	-0.30448213641428	2.05997078722419	2.22106388340164
H	-0.53855819536829	-2.26164233793672	2.00732810828355
C	-0.83723296995660	-0.86558334431118	3.70944171908108
H	-1.07927780919803	-1.53607810608709	4.52216223311844
C	-0.74803889854361	0.54564583651759	3.78574202637419
H	-0.92234277642731	1.15220059324935	4.66338704855098
C	-0.43170486010262	1.02225656328883	2.48870304867238
Fe	-2.20756334115645	0.02335795509621	2.47525240358676
H	-3.51303070598861	2.45317870157467	1.84953185067459
C	-3.67896880500419	1.40628685015939	2.06056118521343
C	-3.88400010378260	0.83712910787862	3.34243821411358
H	-3.63022114146939	0.47960116097096	0.03567872955035
H	-3.89332067913503	1.37209300476213	4.28152851935546
C	-4.05819058753741	-0.56095549298918	3.17807530702770
H	-4.22630613485299	-1.27662980605119	3.97031330388577
C	-3.95973895801059	-0.85588795749599	1.79732976898548
H	-4.03951355302786	-1.83444092328911	1.35022139917728
C	-3.72785325341882	0.36045379997948	1.10479482106294
H	-1.43108738702095	0.71340835593369	-1.15050572415670
C	-1.47448388477009	-0.40107337901961	-3.72562291816627
C	-4.01556693816402	0.14643393894071	-4.67889137592969
C	-2.40520659178476	-1.42697486403432	-3.89403214175805
C	-1.78862561296336	0.90303016537441	-4.10526648232292
C	-3.07974474303754	1.15835723357292	-4.56391740463761
C	-3.67959986275699	-1.16058107648188	-4.35959042584091
H	-3.34469518223957	2.16973008270014	-4.84590736958799
H	-4.39497043057419	-1.96259196865196	-4.47714201185105
H	-5.01167832969867	0.36706589787240	-5.03833230279923
C	-0.78081672960470	2.01371472155385	-4.09741228193299
H	-0.54840529621832	2.30047377266563	-5.12414439592871
H	0.15543907223059	1.74462238974191	-3.61645165905539
H	-1.17661098894352	2.89558717517693	-3.59706240716188
Cl	-1.95948536341882	-3.06368297109922	-3.57279869253511

[1e]⁺ + CN⁻ (C2-CN, is2)

Fe	1.82988588608113	1.27729190396561	0.02464009809542
Fe	1.59990143762942	-1.01409113085058	-0.82915802022903
C	0.17242134439959	-0.65025222248638	-1.96946024524357
C	3.44461140276433	-2.01386263925845	-0.34890800503188
C	2.96439145148264	-2.46847607268788	-1.60408246678838
H	2.53621150132346	-2.06711484579293	1.68397242561482
H	3.49255737939471	-2.41053249098704	-2.54473378944425
C	1.69356876332558	-3.04424722727249	-1.38812803768445
H	1.06154290732377	-3.49107444331179	-2.14333624532020
C	1.38172729899208	-2.93786152097850	-0.01197250218681
C	2.47386583674018	-2.30039066054500	0.63114676974856
H	4.39354266564052	-1.52400923292208	-0.18725982794671
C	2.36192832051625	0.44973287410663	-1.63155417579171
O	2.94896081952422	0.78641209662845	-2.59085042645516
H	3.13221209678873	3.79811457204709	-0.16830974685582
C	3.08959132231405	2.90602828427252	0.44010860077324
C	3.89249169500931	1.76396947700258	0.29325810472756
H	1.49627472296252	3.39028303414759	1.93456168723640
H	4.65874874769563	1.61659448408566	-0.45351901140859
C	3.53167508063865	0.83809442435684	1.30993473354283
H	3.99883177852309	-0.11518525181018	1.49122653021029
C	2.51407315695483	1.41099945437347	2.08639560834916
H	2.02991197331995	0.94697673100926	2.93068859822981
C	2.20961913691249	2.67947622358068	1.54294633975240
N	-0.16317957067865	-0.77031708002942	-3.22169545453386
C	0.76643782243432	-1.24360055314040	-4.24259732796275
H	0.84597955166898	-0.49763431103976	-5.03174759471344
H	0.40534260345768	-2.17548138107717	-4.67587542709196
H	1.74354050516031	-1.40653704794476	-3.80482651385025
C	-1.64169043811632	-1.29414882907664	-0.65388345268884
N	-2.26443292225371	-2.25369589836721	-0.52392772059104
H	0.48615253145004	-3.31142091593323	0.45941443130405
C	0.63636588033168	2.31218047046108	-0.70069817741723
O	-0.14752873544370	3.07868939792750	-1.03036224647918
C	0.28977772107494	0.00572397866855	0.21751153941103
C	-0.77354982951556	-0.14703190531020	-0.90542450032545
C	-0.24932920096704	-0.09188897871358	1.60637785555658
C	-0.55660430030775	-1.25887420284816	2.36313250684089
H	-0.31135689436469	2.04880081824938	2.23443548944639
H	-0.53993227746432	-2.27165268971887	1.99191982181716
C	-0.84766090263086	-0.88693041922379	3.70138248549049
H	-1.09316646320827	-1.56283975167236	4.50857014355070
C	-0.76042892087197	0.52377611166434	3.78702334319038
H	-0.93983398496079	1.12438997032199	4.66772104470887
C	-0.43795065199790	1.00908941025465	2.49470786203774
Fe	-2.21217325286396	0.00814468192574	2.46480373058079
H	-3.51765240657944	2.43903521338592	1.84312457362377
C	-3.68313078195862	1.39093998004770	2.04848428467908
C	-3.89434039125215	0.81558000311938	3.32652510246918
H	-3.62280386731649	0.47388453902381	0.01948337548318
H	-3.90926162244142	1.34629048654065	4.26794995771307
C	-4.06522448251493	-0.58208330306085	3.15494979356183
H	-4.23660640812274	-1.30161015957768	3.94299024079418
C	-3.95885284256582	-0.87056308040179	1.77339109311092
H	-4.03501313478653	-1.84724810103251	1.32158887390473
C	-3.72509064451487	0.34932247553539	1.08760220554620
H	-1.42297235867251	0.70676766239751	-1.15803227376881
C	-1.46661243593518	-0.44523154994024	-3.71513426134883
C	-3.97065007819004	0.23882095888484	-4.67009150577611
C	-2.42081178891035	-1.44838433753219	-3.88402078532362
C	-1.74869557122429	0.86699602771305	-4.08570291459506
C	-3.00088402463285	1.22287703851808	-4.55197624491719
C	-3.67934179515155	-1.07643389769565	-4.35255634770577
H	-3.21077295729691	2.24781553598342	-4.82445850465578
H	-4.43906076651187	-1.83798155352700	-4.47541486726007
H	-4.95630474279094	0.50367770624274	-5.02856178197262
C	-2.11402208788833	-2.89753243131889	-3.65114975658374
H	-1.86176393644405	-3.37708911238941	-4.59938384007870
H	-2.98118515031155	-3.41447635075822	-3.24465791224873
H	-1.28428325601480	-3.05685661063012	-2.96823649024865
Cl	-0.50454646416136	2.05848216442133	-4.00110384857743

[1e]⁺ + CN⁻ (C2-CN, is3)

Fe	2.02166662639921	1.51602201627138	0.04664242191108
Fe	1.43410325048439	-0.73978565620127	-0.84375585296043
C	0.29380116130466	0.01407752496414	-2.15237195096331
C	2.95339291764226	-2.24473414583099	-0.61577563671286
C	2.03533373250155	-2.61422092380207	-1.61944536529642
H	2.69510838896258	-1.84065963947443	1.55657771835443
H	2.27041526757580	-2.80555376985985	-2.65585014930197
C	0.75242236078878	-2.70292104244200	-1.01061431207035
H	-0.16814142692244	-2.99456827700890	-1.49111646346799
C	0.89521419763882	-2.39540724576095	0.36076744667256
C	2.25428267646007	-2.10134541893494	0.60691019265633
H	4.01404640015919	-2.09075048364209	-0.75498021274756
C	2.75396048047101	0.37832472292088	-1.36913831016195
O	3.70225988494070	0.48354047841172	-2.05211295192941
H	4.41291028308660	3.07862875197806	-0.15047713917424
C	3.75590898400575	2.60147292654454	0.56190225571359
C	3.88062927382658	1.29258919038163	1.06972435940053
H	2.25175305340562	4.19545918805439	1.01838767278688
H	4.64690907304209	0.57869154317527	0.80307228737690
C	2.82948768353766	1.06740434270243	1.98888327903360
H	2.68138437244296	0.16967802334692	2.56460626091436
C	2.04437264642255	2.23981191859449	2.05436649742701
H	1.16205742384330	2.38627868006544	2.65866199886275
C	2.60846571933433	3.18668900256012	1.17412802196490
N	0.06771500294597	0.02489257639520	-3.43627214358556
C	-0.93338815540381	0.83858925117589	-4.12705718056067
H	-1.75330125943302	0.21440751915158	-4.47898051586254
H	-0.46467573201506	1.32064399783229	-4.98313730765113
H	-1.32702425959929	1.61261537452803	-3.47671588719014
C	-1.89941141280599	0.14389223338995	-1.26893103775346
N	-2.92163149679390	-0.34717808470220	-1.46681267346625
H	0.09591904736831	-2.36666541309463	1.08222237667300
C	1.50198524995195	2.64174151573490	-1.17979429461659
O	1.23291583039017	3.45977722849319	-1.93485993744775
C	0.27796319769101	0.53792955172810	0.04546843617071
C	-0.59233775544164	0.79442328445691	-1.19843860737460
C	-0.43504015429440	0.53724643568895	1.33464748168171
C	-0.03939355442871	-0.06933945667445	2.56150733056607
H	-2.10018499596521	1.98196737758960	0.94692580775069
H	0.76294459725355	-0.78085643591494	2.68063781395374
C	-0.82769543022149	0.45133032758690	3.61838854359603
H	-0.741719532510082	0.19032984718463	4.66404822943844
C	-1.77195380215293	1.34284230347457	3.05215875503183
H	-2.53337073664045	1.89331544546803	3.58679405996984
C	-1.54899571914830	1.37317801578395	1.65128229396118
Fe	-2.01461143660832	-0.54433170298997	2.29756708721414
H	-4.62629735775550	-0.48610679085208	3.37345229615839
C	-3.91525950113796	-1.11373859260115	2.85507381622948
C	-2.95158034706870	-1.95772993907318	3.46334286640295
H	-4.35590479611115	-0.70168770756338	0.70917621563234
H	-2.79830069471554	-2.08701557959186	4.52540094986911
C	-2.21772123300982	-2.59537546782902	2.43229671012919
H	-1.41497593224973	-3.30500974469613	2.57675099893042
C	-2.72180986267109	-2.14178368462526	1.18726768077292
H	-2.36729270866079	-2.43753950424987	0.21159144204701
C	-3.77164051970836	-1.22483643672133	1.45023213673758
H	-0.79703649230116	1.84480937180362	-1.45045696329990
C	0.80963807832992	-0.84446857460646	-4.29703169311079
C	2.22246710991047	-2.60701378926919	-5.89901429543368
C	1.97397733425513	-0.40300776997023	-4.92323215200901
C	0.31776929104313	-2.12233108674651	-4.55378800798801
C	1.01935545483756	-3.01453375866421	-5.34339438539088
C	2.68142734893258	-1.31600941249392	-5.70371035300644
H	0.63109926261474	-4.00798047371691	-5.52092953318247
H	3.60084466072260	-0.99721103880751	-6.17872430930656
H	2.78908032490888	-3.29824143031277	-6.50848474338378
C	2.43347587478523	1.02245794895817	-4.85823205019700
H	3.51910434666682	1.08123751352613	-4.81730912573756
H	2.03656711272620	1.56846211599478	-4.00827003664794
H	2.11310891721903	1.54548958655584	-5.76183690795670
Cl	-1.21688480246412	-2.59928765374795	-3.91612125504576

[1e]⁺ + CN⁻ (C2-CN, is4)

Fe	2.04188248777280	1.49317120276995	0.03532617475719
Fe	1.42582573523071	-0.76050340284794	-0.84547054200361
C	0.28731741150168	0.01330727417943	-2.14591174365253
C	2.91617467145899	-2.29622150019835	-0.60654092741979
C	2.00671563019820	-2.64205434891274	-1.62633023642742
H	2.63384516258386	-1.89735521501893	1.56363955397132
H	2.25250481877406	-2.83078452007828	-2.66058354870183
C	0.71382436513948	-2.71088917114871	-1.03674391426944
H	-0.20414273983892	-2.99236617257083	-1.52953925390909
C	0.84146829402854	-2.41345697483833	0.33882683706488
C	2.20247378776388	-2.14654700956095	0.60644760508233
H	3.98108792995331	-2.15958627328999	-0.72982105307708
C	2.78155281519286	0.32862519321764	-1.35273038545669
O	3.74457176795141	0.40276316974371	-2.01624914000293
H	4.42706117932405	3.06507559722145	-0.16188397596333
C	3.76812924674454	2.59054984465245	0.55053344097792
C	3.89657183116600	1.28660524455603	1.06952689323968
H	2.25342964205840	4.18115234489422	0.98623847575183
H	4.66785712540415	0.57481090944003	0.81215834121411
C	2.84048175384973	1.06239727831089	1.98306053333525
H	2.69299528552679	0.16723123833856	2.56327156688704
C	2.05056870471491	2.23301030990324	2.03631607432505
H	1.16445855784585	2.38040687402468	2.63479582518428
C	2.61456658132657	3.17564504491450	1.15226045407676
N	0.03171575348060	0.00468672992587	-3.42350690725325
C	-1.00751170401625	0.78272684916321	-4.09916917420327
H	-1.85081581151474	0.14394149243742	-4.35985837170038
H	-0.59464910628003	1.20828960528926	-5.01122123559115
H	-1.35604452605289	1.59758901348396	-3.47276465826829
C	-1.89818909803044	0.14997757523545	-1.24378800737311
N	-2.91901298211301	-0.34567018993878	-1.43984090507818
H	0.03271895088757	-2.37460235133806	1.04944026235711
C	1.54931262297511	2.59942435336932	-1.22563693014396
O	1.29748059195526	3.40503131753433	-1.99825877697340
C	0.29063671140830	0.53088644210004	0.05091220396907
C	-0.58846925654814	0.79633804768365	-1.18412148062530
C	-0.41448766297545	0.53392156321278	1.34500001129931
C	-0.02165139827650	-0.08304627091517	2.56745345749875
H	-2.05637932315037	2.00770401755258	0.97166041505834
H	0.76880004638443	-0.80880392699741	2.68109368791966
C	-0.79175056384693	0.45102443657138	3.63156124192167
H	-0.70176576924968	0.18761802941194	4.67628556793074
C	-1.72399066206087	1.36061637613044	3.07402434522418
H	-2.47073581588290	1.92461774427766	3.61528624110417
C	-1.51167836708845	1.38773144989865	1.67137536305406
Fe	-2.00972257979855	-0.52043078837550	2.32225092380092
H	-4.60467170666703	-0.40381075404545	3.43009828889605
C	-3.91531909165965	-1.04755441425823	2.90238244920726
C	-2.96402760283145	-1.91456344145274	3.49782032943687
H	-4.37179461215439	-0.62172309766609	0.76231996700479
H	-2.80103727032803	-2.04869181099663	4.55779300800951
C	-2.25786701327107	-2.56783630990264	2.45739190032734
H	-1.46967892066912	-3.29571487486080	2.59097807857652
C	-2.76740879906903	-2.10197966367943	1.21950540249730
H	-2.43281657417724	-2.40659073668545	0.23969082820664
C	-3.79163525432379	-1.16024341378278	1.49573038582179
H	-0.78823543049460	1.84805209057452	-1.43547527516418
C	0.78374987542297	-0.84668310724902	-4.29077958839446
C	2.29829283131542	-2.46761220617208	-5.94090100853367
C	1.93920845316329	-0.35712909668323	-4.89198181434986
C	0.32627529220629	-2.13153137261540	-4.57841253985900
C	1.11280503454778	-2.93564392114014	-5.40011754948210
C	2.71347107878316	-1.16562380735419	-5.70506739352243
H	0.78402880963373	-3.94411164894110	-5.61840792346337
H	3.61829005956007	-0.78093952376843	-6.15483257414667
H	2.89747855404078	-3.11203028680017	-6.57017121913578
C	-0.99455609737398	-2.64122239726574	-4.08227275531579
H	-1.35506348171875	-2.11641416172649	-3.20126342693891
H	-0.93446618324862	-3.70201541954210	-3.84248922373949
H	-1.75303573239827	-2.52722942326707	-4.85922249892943
Cl	2.37676368583359	1.29782334586616	-4.67432417592044

[1e]⁺ + CN⁻ (C2-CN, is5)

Fe	1.71899345059776	1.62490278709446	-0.34632156631444
Fe	1.31004134993823	-0.74758467602997	-1.03151494519952
C	0.14541416971163	-0.06977263119353	-2.35659669621235
C	2.86376633227797	-2.24118183691271	-0.75638933297279
C	1.95653056281862	-2.63860703399446	-1.75672612907378
H	2.58897354518390	-1.80236120679288	1.40975775586179
H	2.20042310323248	-2.85226225986420	-2.78638710200601
C	0.66860244107072	-2.72049843842608	-1.15554562362988
H	-0.24636968397104	-3.03438711995590	-1.63477721806740
C	0.80071196553429	-2.37782837823470	0.20947005485926
C	2.15664254963729	-2.07129482892505	0.45831824277458
H	3.92460063829061	-2.08819675965954	-0.89181684025726
C	2.67558091297267	0.38187082426675	-1.49582144495168
O	3.67896466136090	0.41525882578871	-2.09707928428798
N	-0.09695740537066	-0.11450686178263	-3.63559491295763
C	-1.18854018396289	0.57027955762059	-4.32982504849527
H	-1.96617039771607	-0.14060493256784	-4.60611342094500
H	-0.79881768348909	1.03595404503207	-5.23262429086543
H	-1.61906643876572	1.34585882762249	-3.70494192138021
C	-2.03614170214688	-0.13026344977245	-1.42409910888690
N	-3.00404711409469	-0.73917151296826	-1.56082361628823
H	0.00041574760209	-2.32626748219117	0.92864566266336
C	0.10388742646443	0.47417682126986	-0.17064137839265
C	-0.79640160060319	0.64477123049701	-1.40599265879434
C	-0.56004297354662	0.54005342810315	1.14085062777763
C	-0.06890305702718	0.07676945836817	2.39654881143965
H	-2.34434602225575	1.82102829376045	0.70417914200968
H	0.78295567685644	-0.57127924186020	2.53847723835578
C	-0.85678825612684	0.63059283001579	3.43745838599266
H	-0.71425006518112	0.46975776097081	4.49691263612848
C	-1.88668973383797	1.39698686186648	2.83936279534118
H	-2.66626869771546	1.93602685696089	3.35930274328762
C	-1.72102969364491	1.31897953187288	1.43238356778947
Fe	-2.02362056193183	-0.55430198568505	2.25137601304336
H	-4.59788145209428	-0.55472625133465	3.41487136013327
C	-3.87075671864859	-1.18196865981679	2.91866761610325
C	-2.84249927560918	-1.92533982131902	3.55264618747125
H	-4.40104542802497	-0.95612861646231	0.76358350178769
H	-2.64931542607759	-1.96596892542818	4.61520675743992
C	-2.10861965843347	-2.60100995809083	2.54589279867753
H	-1.26198905792093	-3.25245647434600	2.71103127286649
C	-2.67888129251773	-2.27042628074772	1.29045295872511
H	-2.34846963013249	-2.62691842541982	0.32649359992774
C	-3.76597362922035	-1.38980728909390	1.52125128426558
H	-1.09351375276354	1.66670276719936	-1.67854923959156
C	0.72791639100042	-0.92129408520312	-4.47892382850407
C	2.38492303770160	-2.46259556440068	-6.07025372307507
C	1.87423881374916	-0.37203396864650	-5.04475776576473
C	0.35664640000403	-2.23300622809084	-4.76916382063043
C	1.21210317294728	-2.99456813602924	-5.56244795953120
C	2.71875447456243	-1.13865087243460	-5.82767713904613
H	0.94905523714991	-4.02201525653898	-5.78080553138495
H	3.61602055379451	-0.70576665787657	-6.24765411588761
C	2.52315303633933	1.08273989305420	1.11579231216508
O	3.11999309761565	0.84346881653084	2.06106399537704
H	3.22645189970704	3.06445769400654	-2.38552559415802
C	2.48139449216830	3.19433622102245	-1.61514836742620
C	2.74322466217154	3.48031286355580	-0.26450090335277
H	0.57576045718766	2.90644915718722	-2.72662098995443
H	3.71835176744144	3.63191166846089	0.17596358417631
C	1.48830703997540	3.56388058219055	0.41519380815683
H	1.34138844889436	3.79323953098231	1.46077542355736
C	0.47286569374546	3.32690173197443	-0.53030577725004
H	-0.58673983572921	3.32928615632338	-0.31823743373565
C	1.08053804572832	3.08709687801477	-1.78948414633300
H	3.04020579504869	-3.07396857730849	-6.67602961525987
Cl	2.22062081579595	1.30322019957167	-4.81745481294918
C	-0.94107086487267	-2.82031706155377	-4.29915143333147
H	-1.33625132959618	-2.33567126603339	-3.40994362175442
H	-0.82935955430771	-3.88185262163271	-4.08297707240170
H	-1.69810268894177	-2.72675346656019	-5.08030270685366

[1e]⁺ + CN⁻ (C2-CN, is6)

Fe	1.70057925179199	1.63032759428374	-0.34176207383624
Fe	1.30899561639526	-0.74488929460070	-1.02425139100801
C	0.14281163465810	-0.07382003907900	-2.35293209562921
C	2.86728774242533	-2.23609205819136	-0.77676564674006
C	1.93584091157913	-2.63804713994707	-1.75214355242765
H	2.64404638129157	-1.78598555938848	1.39389911725560
H	2.15641590485123	-2.85601690719076	-2.78630200697737
C	0.66156187213014	-2.71473985338319	-1.12037268896961
H	-0.26489431155803	-3.02263735955380	-1.58017894287517
C	0.82816104702183	-2.36710885630875	0.23952182190705
C	2.18910725822950	-2.05898082711491	0.45426430274079
H	3.92480118113212	-2.08574089544010	-0.93839823006167
C	2.66437399414080	0.39206839907746	-1.48801384328080
O	3.66699162105061	0.43984504015450	-2.09295476855003
N	-0.08197643810629	-0.09394503826031	-3.63598320948153
C	-1.15623234279137	0.61887127123409	-4.33064723612209
H	-1.93534739531349	-0.07556240776771	-4.64037442631947
H	-0.74527158637417	1.10527097084808	-5.21329392649082
H	-1.59102972589879	1.38152651548624	-3.69304625666088
C	-2.04203423472796	-0.14890865938262	-1.42457516405800
N	-3.00997773594863	-0.75822121621132	-1.55618208393618
H	0.04452835532473	-2.31166494341011	0.97648749864964
C	0.09333204519769	0.46706124710490	-0.16563952144218
C	-0.80580566036981	0.63209309157206	-1.40268556222083
C	-0.57028536163578	0.53342794477792	1.14609352979523
C	-0.07301145110950	0.08331062988873	2.40445822435212
H	-2.36824595552986	1.79333544983754	0.70330605711634
H	0.78556895879747	-0.55512811415682	2.55000729426590
C	-0.86684758421156	0.63388150053674	3.44237927774269
H	-0.72233961515628	0.48025957051089	4.50261377636987
C	-1.90491806739170	1.38611844239434	2.84038475233180
H	-2.69023866886590	1.91933273650048	3.35762730351394
C	-1.73894513392160	1.30238863298382	1.43389549214389
Fe	-2.02055048467804	-0.56927947827650	2.26108260969558
H	-4.59692344132972	-0.59290127631050	3.41910780743532
C	-3.86173091321299	-1.21422759208954	2.92733652602353
C	-2.82667003257189	-1.94323031545211	3.56686290627499
H	-4.38891989966359	-1.00285581122167	0.77002407097936
H	-2.63516735981699	-1.97683463758638	4.62998040819491
C	-2.08290846143326	-2.61495461201088	2.56462615270330
H	-1.22880017380031	-3.25530138822995	2.73448156700200
C	-2.65378842190613	-2.29596855897603	1.30633850312294
H	-2.31540391262293	-2.65052836176480	0.34440764023733
C	-3.75150332763124	-1.42703841469122	1.53106605024559
H	-1.10878705445810	1.65358127076216	-1.67034541274351
C	0.74503942496999	-0.89334575534570	-4.48622051058225
C	2.32129497422212	-2.50715690427246	-6.09376218453012
C	1.90032094755435	-0.35957503167515	-5.05519910292697
C	0.35466652834382	-2.19586265494948	-4.78504590825196
C	1.13779364049586	-3.01342438096387	-5.58001359001285
C	2.68892004547284	-1.19647704815263	-5.84212085703841
H	0.82769660180450	-4.02750064359051	-5.79117834238638
H	3.60132923555320	-0.80363792921045	-6.27282017863326
C	2.51091473801254	1.09221483677699	1.11872156779455
O	3.11191099249550	0.85695214546351	2.06212372882808
H	3.17455122987713	3.09953135422280	-2.39487971110674
C	2.43971068807991	3.21712127743125	-1.61221155346529
C	2.71995599359603	3.48977885290899	-0.26261319511567
H	0.51665258047859	2.94724544338344	-2.70034317064174
H	3.70068298614885	3.64214749621290	0.16480785995659
C	1.47408990763145	3.56365020414844	0.43488995857449
H	1.34132077742031	3.78335896565176	1.48445010048703
C	0.44586246796593	3.32915302475817	-0.49674532541437
H	-0.61093613121114	3.32512869110325	-0.27163716671698
C	1.03714161485760	3.10657414111697	-1.76733126603674
H	2.94952739578820	-3.13883743569752	-6.70728684237547
C	2.26919928456198	1.08599376114627	-4.91016081586566
H	3.34846897516383	1.21491591483679	-4.96054206935703
H	1.92205718226931	1.52853807488105	-3.98162964403467
H	1.83333220355641	1.66214853456187	-5.72934233123447
Cl	-1.13998230909072	-2.81180862670372	-4.17306510018211

[1e]⁺ + CN⁻ (C2-CN, is7)

Fe	1.86644307714125	1.43481425948488	-0.00572471787905
Fe	1.37114952737694	-0.92315553591149	-0.61579150055114
C	0.04433784283508	-0.44174436262248	-1.85910694529125
C	3.01632144980325	-2.24587830926866	-0.20645415981134
C	2.21427008805057	-2.76400824465348	-1.25075292588202
H	2.55752890316923	-1.78949958646100	1.91768686647181
H	2.54642013089579	-2.99358939817792	-2.25195773206156
C	0.91098836299668	-2.96333471020240	-0.72921549679548
H	0.06334464057764	-3.35879418796808	-1.27117531982877
C	0.91457525951086	-2.57196925252700	0.62964710022844
C	2.22020644265384	-2.13059292514236	0.95209799108605
H	4.06227528359706	-1.98390352617738	-0.28210354188829
C	2.51778397679466	0.22863630964003	-1.40787226893487
O	3.33678728726761	0.33849088464700	-2.24200647206744
H	4.17193163592484	3.06698762135738	-0.46884618411130
C	3.57878537415528	2.62266544818979	0.31706671156981
C	3.78480789143730	1.36030963487371	0.90928039413377
H	2.03468293442379	4.18798366483277	0.74170813937140
H	4.56125780402099	0.65598916099740	0.64698042712406
C	2.79706196420621	1.16771661760087	1.90614650415355
H	2.70967548645753	0.31096067211411	2.55323579376168
C	1.97286598608720	2.31354485339120	1.93478316346921
H	1.12411911339524	2.47499337908665	2.58248437957392
C	2.44394612897519	3.20951262480705	0.95194979325855
N	-0.28491649568435	-0.67174144460293	-3.09925453900359
C	0.53190028001289	-1.50938800204697	-3.97230597785534
H	0.48977680653044	-1.12447975733596	-4.98861342595917
H	0.15492240426321	-2.53187098274444	-3.96775770258754
H	1.56052785098816	-1.49849498889103	-3.63078332598503
H	0.06931874978282	-2.60185251122554	1.29863319922762
C	1.25288242345789	2.44084712929553	-1.29631393131814
O	0.99106756829695	3.21180913279728	-2.09920897582023
C	0.21430116583589	0.40366086876969	0.22791049357552
C	-0.81902434850048	0.33464875686140	-0.91264110806398
C	-0.41351268733155	0.47817068000899	1.56292913396958
C	-0.05542531451355	-0.18571669362071	2.76913209882841
H	-1.96786675005141	2.05936200703764	1.23069281386270
H	0.69887672487603	-0.94977715727098	2.87418030117295
C	-0.84161359870573	0.32152715145093	3.83476754511104
H	-0.79379362217057	0.00327779833137	4.86667894475743
C	-1.71392697571938	1.29990792175642	3.30092289765905
H	-2.45056391093920	1.86910086358155	3.85061420653644
C	-1.46447885390850	1.38459437907933	1.90837114777306
Fe	-2.05942604846170	-0.51079414850037	2.40937673862934
H	-4.82566453604588	-0.12965392481688	2.83126380931376
C	-4.08557782389567	-0.85772515191444	2.53137508883101
C	-3.38370869181995	-1.73760783447626	3.39494271964284
H	-3.97745311771201	-0.57779521050256	0.31903300867623
H	-3.49706312703914	-1.79795322506947	4.46798679950039
C	-2.50185637739015	-2.51679580864608	2.60473762533752
H	-1.82736433117637	-3.27843476732421	2.96974261551042
C	-2.65937214579651	-2.11908494207854	1.25278261072634
H	-2.12765868503878	-2.52726414396202	0.40617723292952
C	-3.63592194860013	-1.09173604253364	1.20694484181569
H	-1.62028631043991	-0.35596504243223	-0.60725107601270
C	-1.51847997114245	1.54712324584730	-1.33736168428087
N	-2.08414884407561	2.51578656349064	-1.59993832647706
C	-1.50419788458950	-0.20097803181446	-3.67997051709271
C	-3.89179320500363	0.69275725784261	-4.75835731395984
C	-2.69743833712951	-0.86670652165769	-3.41159452382432
C	-1.49112004769398	0.90262411609837	-4.53237347410670
C	-2.70416347313667	1.33725835721264	-5.05844462115844
C	-3.89773674710190	-0.42237108120218	-3.93508675765148
H	-2.71341882761097	2.20333084583861	-5.70820894821207
H	-4.81820140099262	-0.94249570005873	-3.70935480964884
H	-4.82364745213741	1.05369754423351	-5.17245484326041
C	-0.22331443427015	1.61286392845631	-4.89940770095976
H	0.09200857916917	1.32665802520093	-5.90472825729004
H	0.59972040434866	1.39438487632042	-4.22423255175483
H	-0.37683413000034	2.69088636597760	-4.90267867943429
Cl	-2.68880309349044	-2.28908679267130	-2.42805080076921

[1e]⁺ + CN⁻ (C2-CN, is8)

Fe	1.87758341473926	1.44161366509209	0.00247381089842
Fe	1.36703638371962	-0.91093522201213	-0.61647541795320
C	0.03942931343880	-0.42573211727898	-1.85529494935604
C	3.00462927203984	-2.24766291936203	-0.21761350633274
C	2.19314447231636	-2.75714091557305	-1.25850182226250
H	2.56122089759667	-1.79077191234601	1.90969029605406
H	2.51819919939835	-2.98828803422030	-2.26164216695694
C	3.59894326421621	-2.94685778690173	-0.73000830367273
H	0.03778248675207	-3.33815268798327	-1.26686035907708
C	0.90489936257645	-2.55784164617960	0.62949033258680
C	2.21563663513553	-2.12754572379440	0.94552502296111
H	4.05224746869789	-1.99416963969474	-0.29865964140190
C	2.52267348548344	0.23791824342103	-1.40324501761524
O	3.34588541059891	0.34171348172404	-2.23328115005276
H	4.19313208740334	3.06000488816976	-0.45853702164764
C	3.59894326421621	2.61646659973578	0.32704472882728
C	3.79738476191043	1.35002642177628	0.91315151237601
H	2.06767319180788	4.19096837283951	0.76350522185258
H	4.56815634755251	0.64139204630803	0.64569360059841
C	2.81112888458144	1.16001307353411	1.91189001775510
H	2.72089501428753	0.30183253399238	2.55665791322692
C	1.99526130617119	2.31159619462240	1.94767777617304
H	1.14962163108984	2.47662935006458	2.59854585723388
C	2.47019781763028	3.20848533263499	0.96782812744783
N	-0.30560040390135	-0.67932390470589	-3.08611327417745
C	0.52366194018807	-1.49839131738848	-3.96693826312397
H	0.46112597349532	-1.11597885585524	-4.98284219893762
H	0.17857803690125	-2.53179756312777	-3.95814981956039
H	1.55497873233193	-1.45862534047147	-3.63598777451045
H	0.06335589523338	-2.58314428741591	1.30333865490114
C	1.27276763823490	2.46926343050280	-1.28019203584267
O	1.02328126980287	3.25918371213308	-2.06678864823564
C	0.21854226088188	0.42022272511788	0.23179799128813
C	-0.81793858396703	0.35745078503098	-0.90685358415739
C	-0.40530576478863	0.49690185547673	1.56855266747044
C	-0.04539724661910	-0.16749900239027	2.77395969934848
H	-1.95260803171981	2.08587387188139	1.24166836050155
H	0.70491166660097	-0.93586181218297	2.87633890397446
C	-0.82219666704340	0.34685972483449	3.84309653436218
H	-0.77047971661842	0.03054683006352	4.87542020550274
C	-1.69184746588414	1.32911357555643	3.31203103366646
H	-2.42213168534529	1.90370844855821	3.86458062077324
C	-1.44969968423254	1.40929770583179	1.91791789504294
Fe	-2.05285309563462	-0.48193838744536	2.42775873104018
H	-4.81440897736662	-0.08259224472759	2.86295567731129
C	-4.08026896236995	-0.81642010570200	2.56253916447009
C	-3.37889046272596	-1.69651355912126	3.42626727585521
H	-3.98027066890780	-0.54549117682693	0.34831544518376
H	-3.48693576335641	-1.75130654772584	4.50013155543977
C	-2.50553644429479	-2.48465000920153	2.63560230723203
H	-1.83370635916717	-3.24865932698348	3.00037449092270
C	-2.66803212410770	-2.09161214464217	1.28298604479816
H	-2.14156236865765	-2.50836367353455	0.43669522204489
C	-3.63851868978213	-1.05834674768011	1.23694520290486
H	-1.62715340937016	-0.32165938790897	-0.59524301598099
C	-1.50887280339906	1.57496033564864	-1.33035643147607
N	-2.07103063741561	2.54625995555747	-1.59010652980839
C	-1.53912359225970	-0.23340095970808	-3.65784698624054
C	-3.89727483147448	0.66938112187020	-4.78532528662998
C	-2.70705193328091	-0.97285577471851	-3.46514376827137
C	-1.55207459864834	0.91296281737915	-4.44438344479581
C	-2.72741600272946	1.37694100728169	-5.00769729067439
C	-3.88474769802173	-0.49212772839952	-4.02957747234631
H	-2.72727990476757	2.27880911785561	-5.60388114662762
H	-4.80338633306511	-1.04527942208825	-3.88226113764148
H	-4.82456607930238	1.02535782885343	-5.21376951397951
C	-2.69911188077824	-2.26994672680223	-2.71226533373421
H	-2.10798133952707	-3.02534987997206	-3.23269395793177
H	-3.71013524911147	-2.65850103505494	-2.60752510861145
H	-2.28095546786724	-2.17222992807239	-1.71167289109516
Cl	-0.08424236208876	1.77716940185151	-4.70710363130674

[1e]⁺ + CN⁻ (C2-CN, is9)

Fe	1.91959963842019	1.58874883694740	0.12175135603573
Fe	1.48225676927762	-0.73410697180095	-0.69332114918508
C	0.13449557119822	-0.20400048432264	-1.91730481454078
C	3.16562449438589	-2.05242254615413	-0.44410805026296
C	2.30719676161805	-2.53118796192955	-1.45807198034646
H	2.83930996954347	-1.67649084193450	1.72273575973679
H	2.57133513749987	-2.70293096598907	-2.49096705889502
C	1.04531355982092	-2.77755316829288	-0.85787711139295
H	0.17543812406336	-3.18603991469539	-1.34707650521192
C	1.13099179210338	-2.44776007991501	0.51241586221048
C	2.44340497076378	-1.99052500148533	0.76938147670720
H	4.20174996134186	-1.77402930495744	-0.57264557814258
C	2.70212004869601	0.46356699107339	-1.29318402597169
O	3.63042714523184	0.62469959022561	-1.98851371710038
H	4.19993928848079	3.31377653649488	-0.08547941680014
C	3.56566052928717	2.80778583175433	0.62770999224775
C	3.77404036094886	1.52331195385746	1.16911648815404
H	1.93971575921138	4.29922987155311	1.01612320996392
H	4.58984113088550	0.85723340415996	0.92710707038473
C	2.72545579627482	1.24636183907433	2.07802741375838
H	2.62640664335780	0.35457562017109	2.67480789198093
C	1.86042702120236	2.36352838072860	2.10411709065569
H	0.95898421418396	2.45811721930057	2.69071867262148
C	2.36888213140481	3.32557764636318	1.20779190763339
N	-0.29678355291756	-0.45512265553744	-3.12407591436855
C	-1.54951538209048	0.05715717807612	-3.68739918998237
H	-1.82310080992245	-0.54260576339232	-4.55126401328140
H	-1.43293820121273	1.09085724237302	-4.00918369009384
H	-2.35546299045748	-0.01353948544777	-2.96005776986388
H	0.32891806266303	-2.52843329142651	1.22783300857766
C	1.44065896176984	2.62444372490458	-1.21134757733000
O	1.29362772016207	3.38410589838189	-2.05243657473117
C	0.28463746524125	0.51992004121696	0.22245519851070
C	-0.71377346703132	0.56204602945658	-0.94397513697904
C	-0.40334982118420	0.45939575035706	1.52858533425080
C	-0.05817688929870	-0.26393347418481	2.70481449029812
H	-2.05618001942666	1.94319794993087	1.21793119281483
H	0.74890564070182	-0.97386290939860	2.79913520033308
C	-0.93694504260391	0.10436034808240	3.75522711119957
H	-0.91849856517901	-0.28455088670829	4.76360277992116
C	-1.85290471157133	1.05372096919967	3.24186601623598
H	-2.65899049495374	1.52497018806895	3.78656660703525
C	-1.53794781953036	1.25934591120657	1.87538642281594
Fe	-2.01073317784929	-0.70534824448345	2.20571564552664
H	-4.79556456292229	-0.63329244379964	2.67635307203433
C	-3.99697996569335	-1.24492169856276	2.28120784647436
C	-3.21086445035369	-2.16720158467719	3.01826461769793
H	-3.94301986428807	-0.66475636365399	0.12698585738769
H	-3.30545057428640	-2.38216614806684	4.07314199133301
C	-2.27453522841878	-2.75319761377105	2.13017047997196
H	-1.53530072973799	-3.49824912974831	2.38830300641998
C	-2.48134041383002	-2.19247185604762	0.84358208905989
H	-1.93561516662663	-2.44430689326380	-0.05564207227535
C	-3.54468884537010	-1.25880770426046	0.93772620929173
H	-1.57012266145306	-0.09296793715459	-0.71034784672998
C	-1.30322303692604	1.84457960269208	-1.31632767648015
N	-1.78107318461743	2.86303894571849	-1.56471439396969
C	0.48232709402821	-1.27078767301328	-3.99610730699904
C	2.05868678651532	-2.83167093462734	-5.64482441383781
C	1.54752996941793	-0.70728070677750	-4.68989246469358
C	0.13864017866066	-2.60842152413051	-4.18962367896341
C	0.95570526979112	-3.38055084016951	-5.01136946480740
C	2.35350337697085	-1.48416710386664	-5.50383058422148
H	0.71689565630828	-4.42662054083026	-5.15731842482561
H	3.18861701909952	-1.04098731625941	-6.02843348124624
H	2.68503885165031	-3.45046866751682	-6.27332833312918
C	-1.10665780579683	-3.20162734378461	-3.59690507507110
H	-1.43473166679620	-2.69343553463432	-2.69193120682932
H	-0.96314543346323	-4.25522895055538	-3.36102400459899
H	-1.92841490500975	-3.14058314599454	-4.31373978594523
Cl	1.82546156863693	0.99188710585331	-4.58453988017728

[1e]⁺ + CN⁻ (C2-CN, is10)

Fe	1.90650552663181	1.63403796571305	0.18163228111640
Fe	1.49654302382815	-0.67263789395718	-0.69315094179687
C	0.14442925079275	-0.14972897657858	-1.91567145836265
C	3.21032172218034	-1.96599430721015	-0.53074417471606
C	2.30888881711553	-2.45740622068828	-1.49776928912949
H	2.99287581643141	-1.60776807055378	1.65347828157334
H	2.52507408359477	-2.62417761039119	-2.54262802921458
C	1.08171328636387	-2.72241841351872	-0.83448681364846
H	0.19427970493252	-3.14188762562259	-1.27976907039929
C	1.23521131713913	-2.39542821025592	0.53017766548321
C	2.55026532670962	-1.91697364761244	0.71958873453663
H	4.23422632154426	-1.67248435495915	-0.71253089927283
C	2.67273042608537	0.56906147698558	-1.28872090787719
O	3.57385538872113	0.77577856848812	-2.00957167291343
H	4.21354499296519	3.33208724983892	0.02265591399373
C	3.57122512970557	2.81628091800325	0.72140350173152
C	3.75843878979507	1.51378251622778	1.22704581839291
H	1.96794226167340	4.32077911744184	1.14920552334648
H	4.56436534325328	0.84185169619602	0.96823814172683
C	2.70541478618643	1.22943114061703	2.12829691690616
H	2.59141532091572	0.32392427449593	2.70037044499213
C	1.85607322244618	2.35683308528070	2.18247543054064
H	0.95423880858824	2.44793589378603	2.76906210396661
C	2.38164632927481	3.33546710478155	1.31370377077570
N	-0.27877511991458	-0.38117400824476	-3.13048105739719
C	-1.51903635672149	0.16316943508651	-3.69611666226541
H	-1.77300065998466	-0.38744456824312	-4.59716149527499
H	-1.39133523050279	1.21175172295200	-3.95940725846990
H	-2.34237294817882	0.05769719597543	-2.99285793779358
H	0.47385668510907	-2.49668270841892	1.28675715259990
C	1.40549505107693	2.73114401060702	-1.08964011184555
O	1.25008338794719	3.53552075733821	-1.88740350909808
C	0.27767379789663	0.55179909082426	0.24020471880274
C	-0.70830223782915	0.60642615244275	-0.93740088920157
C	-0.42490496776024	0.46535931276519	1.53721688433602
C	-0.07668193000787	-0.25748753924730	2.71333178705862
H	-2.11122258379352	1.90999606575750	1.21650184165844
H	0.74518630622979	-0.94954947576254	2.81204975739806
C	-0.97631784326294	0.08327013259190	3.75512476988407
H	-0.96047947549217	-0.31105218970499	4.76143454750045
C	-1.90921731369993	1.01304238154243	3.23623989802403
H	-2.73291242018675	1.46147348907026	3.77378000980872
C	-1.58274180437970	1.23542273802306	1.87523032791380
Fe	-2.00894338504146	-0.74333225408132	2.18750827043725
H	-4.79033424229178	-0.78766813154995	2.68024984712432
C	-3.97245485119432	-1.35668236361040	2.26142246104215
C	-3.14732852251385	-2.27193906608714	2.96432485290894
H	-3.95559161677164	-0.70984858102212	0.12525881105462
H	-3.22605908739088	-2.52307651595393	4.01250466555969
C	-2.19653362487810	-2.79504461666326	2.05241696191515
H	-1.43013387334545	-3.52124036950502	2.28367777038873
C	-2.43443665890046	-2.20430149572225	0.78514134205974
H	-1.88628847177837	-2.40522443641678	-0.12458654691188
C	-3.53102244713716	-1.31421845443700	0.91472880755949
H	-1.56085947269934	-0.06005120870444	-0.72196018769747
C	-1.30980100492662	1.88809505736453	-1.29267923002218
N	-1.80120181643916	2.90368640665017	-1.52563060149011
C	0.46485172704463	-1.24120672262858	-3.99383997569206
C	1.88546945050964	-3.00291045883992	-5.59122833791745
C	1.54625376094268	-0.76240393072822	-4.72971652891926
C	0.05490237186572	-2.56626891486959	-4.13396448351350
C	0.76130142780772	-3.45805655651349	-4.91823950559530
C	2.25969917974821	-1.67323967977215	-5.50822795889737
H	0.43797560537922	-4.48623060699630	-5.00421398299880
H	3.11658549142944	-1.32248567584951	-6.06963523220320
H	2.45603861985298	-3.69041915547029	-6.20110431448313
C	1.90857214019523	0.69142012700834	-4.77618449041351
H	2.98836411531325	0.82236969013242	-4.79671936447017
H	1.51686689093565	1.26039225969671	-3.93878771188111
H	1.50811450401688	1.13631291718797	-5.68914715690224
Cl	-1.38874354315224	-3.10523193448115	-3.34310622543134

[1e]⁺ + CN⁻ (C2-CN, is11)

Fe	1.61254884807682	1.61502989754159	-0.32046210287871
Fe	1.32382681759187	-0.81029672007640	-0.89116043569831
C	-0.03614197389234	-0.36966386222632	-2.13179497232706
C	3.03947829376283	-2.11405023043865	-0.59342530018515
C	2.18460509944452	-2.62474269924611	-1.59315310265777
H	2.71507169993645	-1.69615202532015	1.56645007954705
H	2.45331891099562	-2.82423907791447	-2.61950203212637
C	0.92187147823154	-2.86135660883750	-0.98706688779911
H	0.05227281923225	-3.28617185954215	-1.46391347469966
C	1.00634942756487	-2.48783558032057	0.37143857214171
C	2.31793035756399	-2.01985997872991	0.61709689031068
H	4.07487084574682	-1.83762168558446	-0.72972012152453
C	2.55859473504829	0.38355817534909	-1.51188093414304
O	3.51203112555830	0.46385589145871	-2.18313797452516
N	-0.40165301591647	-0.62651269104222	-3.35711852521412
C	-1.67912949868474	-0.23900214830641	-3.96370899312591
H	-1.87128330843994	-0.87826046991801	-4.82107898960669
H	-1.64714736349670	0.79501608710293	-4.30286246566107
H	-2.49560717133443	-0.37051539436870	-3.25814049951496
H	0.20642894326425	-2.54763135016321	1.09168191401140
C	0.09438861761834	0.40349748668355	-0.00794831648364
C	-0.94387531747841	0.30200534692063	-1.14134545651707
C	-0.49828320193179	0.43347708383982	1.34292978266958
C	-0.04312312675009	-0.19906619286739	2.53552522547636
H	-2.20867794668299	1.85914582074108	1.06892649454496
H	0.78239263558002	-0.88949070094082	2.61295947972470
C	-0.84086116366540	0.22931645547880	3.62684380353216
H	-0.72954319225735	-0.08514451214396	4.65507331527640
C	-1.81429338786778	1.12595170562665	3.12618797840904
H	-2.58284050176804	1.62263232824273	3.70173464770918
C	-1.61610906299214	1.23966308344240	1.72704533549993
Fe	-2.02253815684565	-0.70087759610609	2.22938387723004
H	-4.76548017133633	-0.59417325237957	2.89025134085218
C	-3.99565497219596	-1.23297371100409	2.48142535847897
C	-3.15565453802518	-2.10334012171390	3.22226131593027
H	-4.08861960819222	-0.79171060609475	0.29589925405247
H	-3.17599925189394	-2.24755171570348	4.29310470436325
C	-2.28158063183117	-2.74894944845622	2.31181652047083
H	-1.52339605344618	-3.47613408866510	2.56640737930024
C	-2.58147932228870	-2.27693025661294	1.00770392589976
H	-2.09663661994871	-2.58794431829874	0.09277595217552
C	-3.63860930288149	-1.33741152657593	1.11322877070591
H	-1.68347342880899	-0.46915329658251	-0.86558485214577
C	-1.76640859812453	1.44742488941691	-1.53353219778199
N	-2.45347261652031	2.32820300093215	-1.81647322163356
C	0.49622511316801	-1.33215856667791	-4.21417227374107
C	2.32117694571484	-2.67156709484063	-5.80656269703694
C	1.52297949329450	-0.63963596806728	-4.84828563659095
C	0.31885516007352	-2.69500887269924	-4.44670669032259
C	1.25662697462881	-3.35168479730586	-5.24000380671870
C	2.45269442308763	-1.30239821130615	-5.62920102696005
H	1.14640581326436	-4.41533944439654	-5.41082946451959
H	3.25712631824169	-0.75531017682250	-6.10077376397939
C	2.45927428285613	1.14214052258133	1.14269017992037
O	3.05841991379741	0.94579984830531	2.09605656227026
H	3.68259007557575	3.61832216306268	-0.11408367893752
C	2.66017369204722	3.46260123407631	-0.42679904980617
C	1.49832615161233	3.58290730933496	0.39475893769048
H	2.87099811103033	2.98716495430666	-2.57942829692778
H	1.48282452918443	3.85112786408065	1.44176853983093
C	0.37079901438896	3.32745330538251	-0.40792408563763
H	-0.65173131769279	3.36472644520106	-0.06782518888423
C	0.81852239387046	3.04401633820101	-1.72578152653876
H	0.20437116120823	2.84947621243206	-2.59043547942081
C	2.22855263273853	3.14432551932166	-1.72653328224408
H	3.04528445678225	-3.20326777845167	-6.40924893351468
C	-0.86004965817166	-3.45621478602575	-3.91525914962273
H	-1.37582723792177	-2.94826630204788	-3.10340460774928
H	-0.55526120560117	-4.43915887330947	-3.55714670466434
H	-1.59013896514068	-3.61687768541336	-4.71128836862135
Cl	1.60338557824391	1.07934831448180	-4.71594556933626

[1e]⁺ + CN⁻ (C2-CN, is12)

Fe	1.59958931530019	1.62909307776008	-0.31159699689704
Fe	1.32620573352501	-0.79811206502565	-0.88217163481558
C	-0.03660905406035	-0.36468209270348	-2.12762340104144
C	3.05295718805241	-2.09100688616666	-0.60340044140898
C	2.18463064890686	-2.61041715323804	-1.58650714623483
H	2.76046191770647	-1.66517560876803	1.56016959921582
H	2.43878024540368	-2.81278422855194	-2.61617869111005
C	0.93219896781442	-2.84958494868710	-0.95938675577175
H	0.05643786924225	-3.27740694939324	-1.42127243581293
C	1.03730875576283	-2.46955605674052	0.39540721743794
C	2.34958910167109	-1.99370189451384	0.61831076486775
H	4.08509310381971	-1.81162292076238	-0.75716150972189
C	2.55170524302740	0.40492180439432	-1.50148005429096
O	3.50165863468574	0.49654483071439	-2.17877284939693
N	-0.38877674829651	-0.59383735625377	-3.36197685233203
C	-1.65231301575949	-0.16806737219846	-3.97537337485772
H	-1.82157976469291	-0.74223649126424	-4.88167666565492
H	-1.61092733499188	0.88701203717207	-4.23981067446297
H	-2.48666286947507	-0.34701357573441	-3.30204696033707
H	0.24934605513255	-2.53188395294603	1.12838481649486
C	0.08872897794809	0.40501499672141	-0.00067524650693
C	-0.94841210201126	0.29888669753308	-1.13480551936354
C	-0.50591338872686	0.43233962822352	1.34926068199897
C	-0.04412951897202	-0.19080591426585	2.54428369134469
H	-2.23651053848889	1.83330924954612	1.06923747618142
H	0.79134410440110	-0.86887800916299	2.62446352308150
C	-0.85153664805332	0.22686802279060	3.63238374637363
H	-0.73881473225001	-0.08481260614539	4.66128509753690
C	-1.83664629104270	1.10838027459475	3.12760106701262
H	-2.61437034945056	1.59427521754639	3.69997443120643
C	-1.63618043242105	1.22335515889353	1.72908616514286
Fe	-2.01517996147033	-0.72248045105698	2.23242195602527
H	-4.76012482353537	-0.65657089623183	2.89126032494153
C	-3.98047605820021	-1.28349418956906	2.48259946664100
C	-3.12850542883857	-2.14226326825220	3.22327865958429
H	-4.07878909920151	-0.84304411660183	0.29711653781188
H	-3.14772779712278	-2.28779837222193	4.29395347036888
C	-2.24449940185419	-2.77431003416623	2.31289877883160
H	-1.47680366248924	-3.49136943339526	2.56766985674441
C	-2.55046293404575	-2.30594818025937	1.00896688064437
H	-2.06229738534071	-2.61064471589266	0.09354845990238
C	-3.62115343593102	-1.38210440675104	1.11459574077647
H	-1.68246068056404	-0.47911441501613	-0.86394772815191
C	-1.77835501106425	1.44326217795127	-1.51509597816335
N	-2.46856639310100	2.32534587422420	-1.78601936774056
C	0.50353944018461	-1.30588483677994	-4.22003988364117
C	2.23942324923735	-2.76197035422172	-5.81039062645238
C	1.54969978343690	-0.64302084330608	-4.85952044536034
C	0.28431366895067	-2.65984527202191	-4.45478252467944
C	1.15102163152961	-3.40145559180231	-5.23732862509026
C	2.42413297411448	-1.40041706740229	-5.63547071586923
H	0.97680571951368	-4.45662085428514	-5.39624157854511
H	3.25594004162141	-0.90570126745917	-6.12075806047254
C	2.45297188367832	1.15979251257233	1.14956438082098
O	3.05570223327201	0.96880484462049	2.10142833564068
H	3.65796652919591	3.64493593624918	-0.10370688884188
C	2.63475980952042	3.48498106945716	-0.41150447292722
C	1.47697825051550	3.59161061879217	0.41771173778616
H	2.83574569624311	3.03538166868215	-2.57093875027378
H	1.46614153556597	3.85085700046315	1.46702710763568
C	0.34624644539885	3.33410140123847	-0.37910656665134
H	-0.67460489108373	3.36179847021138	-0.03328213391130
C	0.78786601529288	3.06762805122619	-1.70296298119011
H	0.16566595363008	2.88977927055427	-2.56624118416092
C	2.19724220618470	3.17693438381414	-1.71171621282746
H	2.93480807008701	-3.33011667035821	-6.41353651355661
C	1.69096490511751	0.84809175029335	-4.80798364335616
H	2.72202289097897	1.14923190824669	-4.98257760213405
H	1.37192486478406	1.27827661445117	-3.86327204979759
H	1.07954111876215	1.30037759000145	-5.59185993871201
Cl	-1.11419302668037	-3.42930281936614	-3.78652728952661