Supplementary Information for:

Towards [NiFe]-hydrogenase biomimetic models that couple H_2 binding with functionally relevant intramolecular electron transfers: a quantum chemical study

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Section 1: Additional information on Ni-containing models of type c, c' and d

1.1 – Relative stabilities of **c** isomers featuring alternative orientation of cyanide, isocyanide and carbonyl groups coordinated to the Fe center in the Ni–Fe core.

Figure S1 reports a schematic representation of **c** and of the isomers of the latter (including **c'**) that feature the alternative possible disposition of ligands in the Fe first coordination sphere. For each isomer, the energy difference with respect to **c** is reported. As anticipated in the paper main text, **c'** is the only model the total energy of which is less than 3 kcal mol^{-1} above the one of **c**.

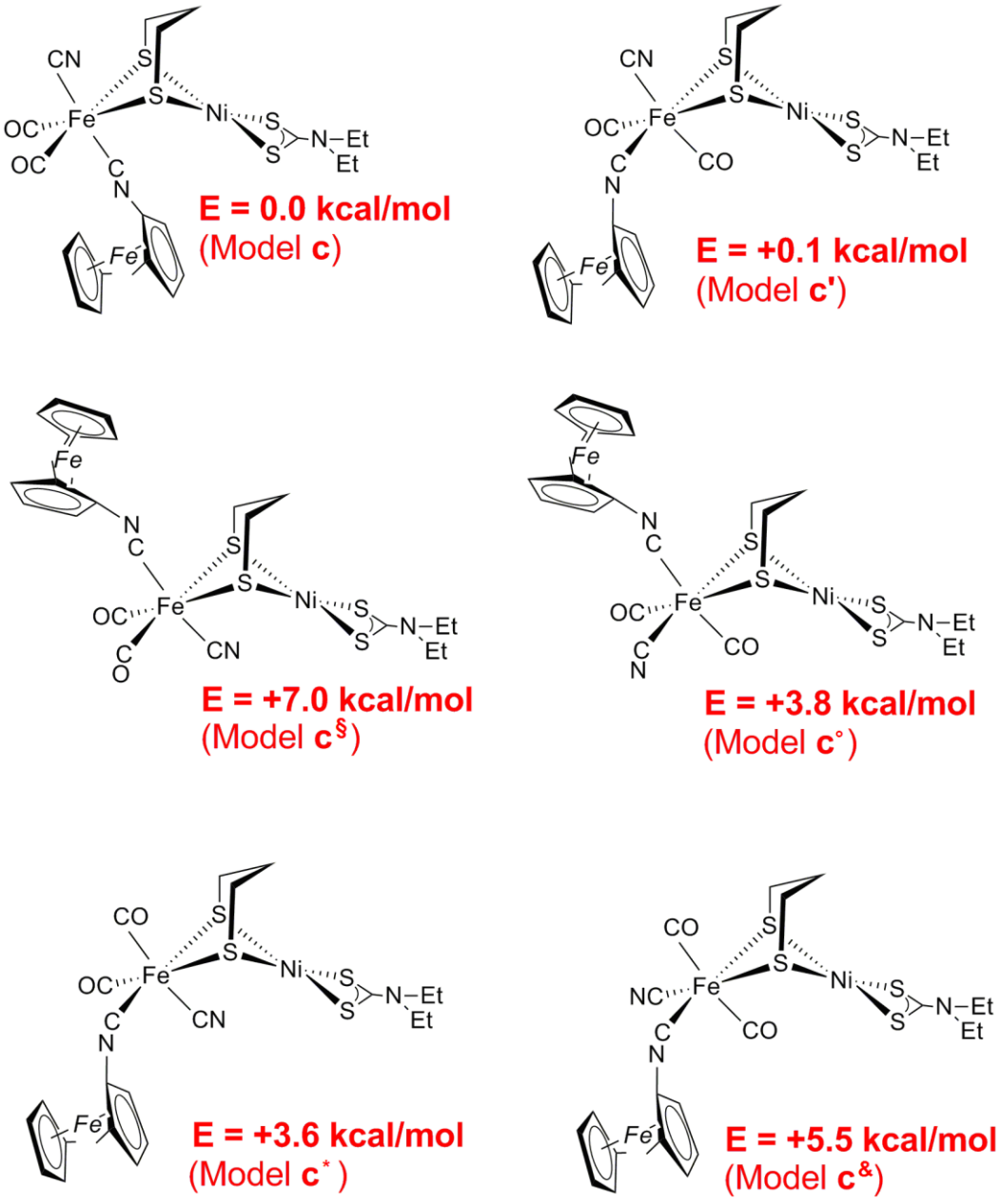


Figure S1.

1.2 – Optimized structures and reactivity of model **c'** and derivatives.

Figure S2 shows the optimized geometry of three minima (**c'**, $\mathbf{[c']^+}$ and $\mathbf{[c']^+\text{-}H_2}$) and one transition state ($\mathbf{[c'_{TS}]^+\text{-}H_2}$). Mulliken population analyses show that **c'** features the *Fe(II)*Fe(II)Ni(II) state, see Table S1. Notably, side-on coordination of H_2 to the Ni center of **c** turned out to be not possible, as geometry optimizations of a complex of such kind invariably led to H_2 detachment along energy minimization. The one-electron oxidation of **c'** leads to $\mathbf{[c']^+}$; notably, overall spin populations and charges of the two portions composing the model are consistent with the *Fe(III)*Fe(II)Ni(II) state for the cationic complex. This implies that the Ni–Fe site does not change redox state, in full analogy with what reported in the paper main text for the $\mathbf{c} \rightarrow \mathbf{c}^+ + e^-$ oxidation.

Then, we optimized the dihydrogen complex $\mathbf{[c']^+\text{-}H_2}$ (see Figure S2). Most notably, H_2 binding to $\mathbf{[c']^+}$ is associated with the oxidation of the Ni center at the expenses of the Fe ion in the metallocene sandwich, an intramolecular redox process similar to the one observed as a result of H_2 binding to $\mathbf{c}^+$. In fact – as reported in Table S1 – the spin population of the dinuclear site increases from 0.01 to 1.01 going from $\mathbf{[c']^+}$ to $\mathbf{[c']^+\text{-}H_2}$. The main contribution to such variation comes from the Ni ion (Mulliken spin population of Ni in $\mathbf{[c']^+}$ and $\mathbf{[c']^+\text{-}H_2}$: 0.00 and 1.10, respectively). Concomitantly, the overall spin population of the metallocene site drops from 0.97 to zero. As far as reaction energies are concerned, H_2 attachment to the Ni center of $\mathbf{[c']^+}$ is disfavored by 9.4 kcal mol^{-1} (a value comparable to the one reported in the main text for the H_2-binding reaction on model $\mathbf{c}^+$: 10.4 kcal mol^{-1}). Finally, the $\mathbf{[c']^+} + H_2 \rightarrow \mathbf{[c']^+\text{-}H_2}$ binding reaction is characterized by a rather small barrier (10.6 kcal mol^{-1}, transition state $\mathbf{[c'_{TS}]^+\text{-}H_2}$ shown in Figure S2), again analogously to the case of dihydrogen binding to $\mathbf{c}^+$ (see the paper main text).

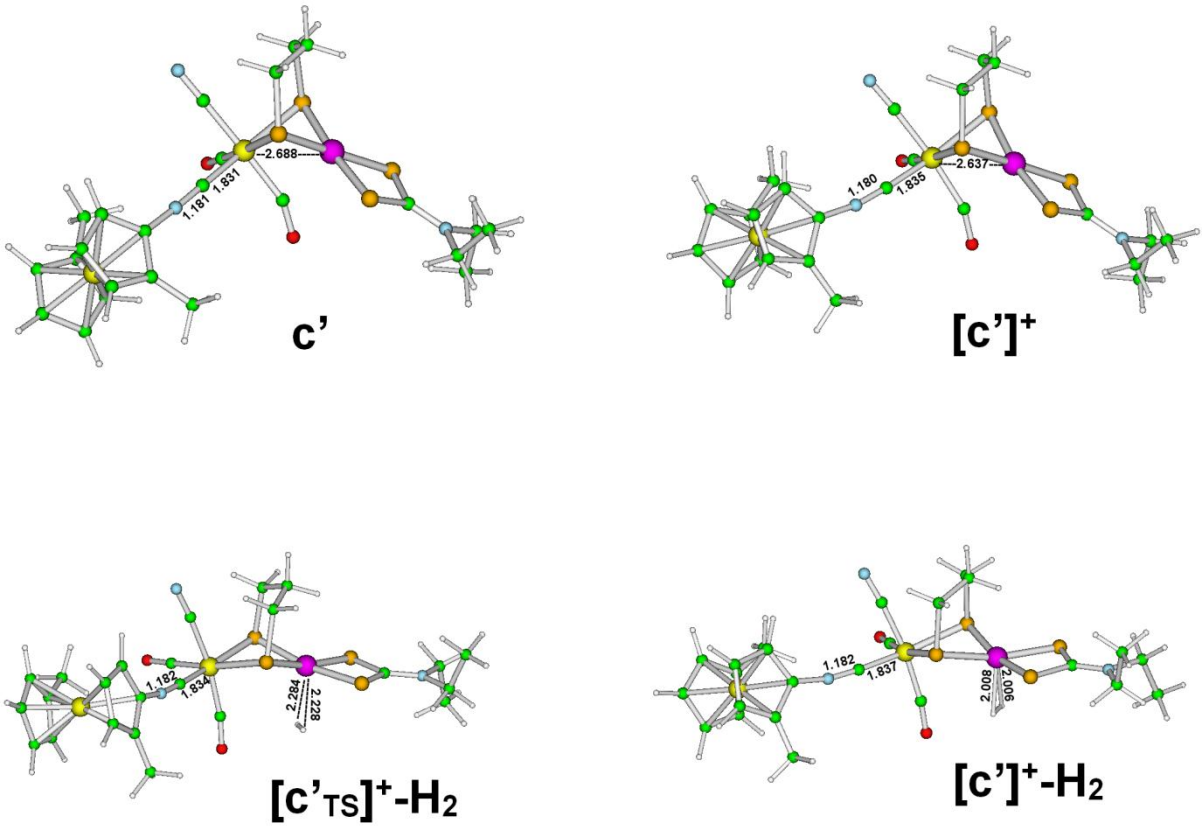


Figure S2. Ball-and-stick representation of models **c'**, **[c']$^+$**, **[c'$_{TS}$]$^+$-H$_2$**, **[c']$^+$-H$_2$**. All interatomic distances in Å. Color code of atoms is the same as in Figure 4 (see main text of the paper). The singlet-triplet split for **c'** and the doublet-quartet split for **[c']$^+$** and **[c']$^+$-H$_2$** are: 14.8, 20.0 and 23.7 kcal mol^{-1}, respectively.

1.3 – Optimized structures of the Ni-containing models featuring dtma as a bridging dithiolate

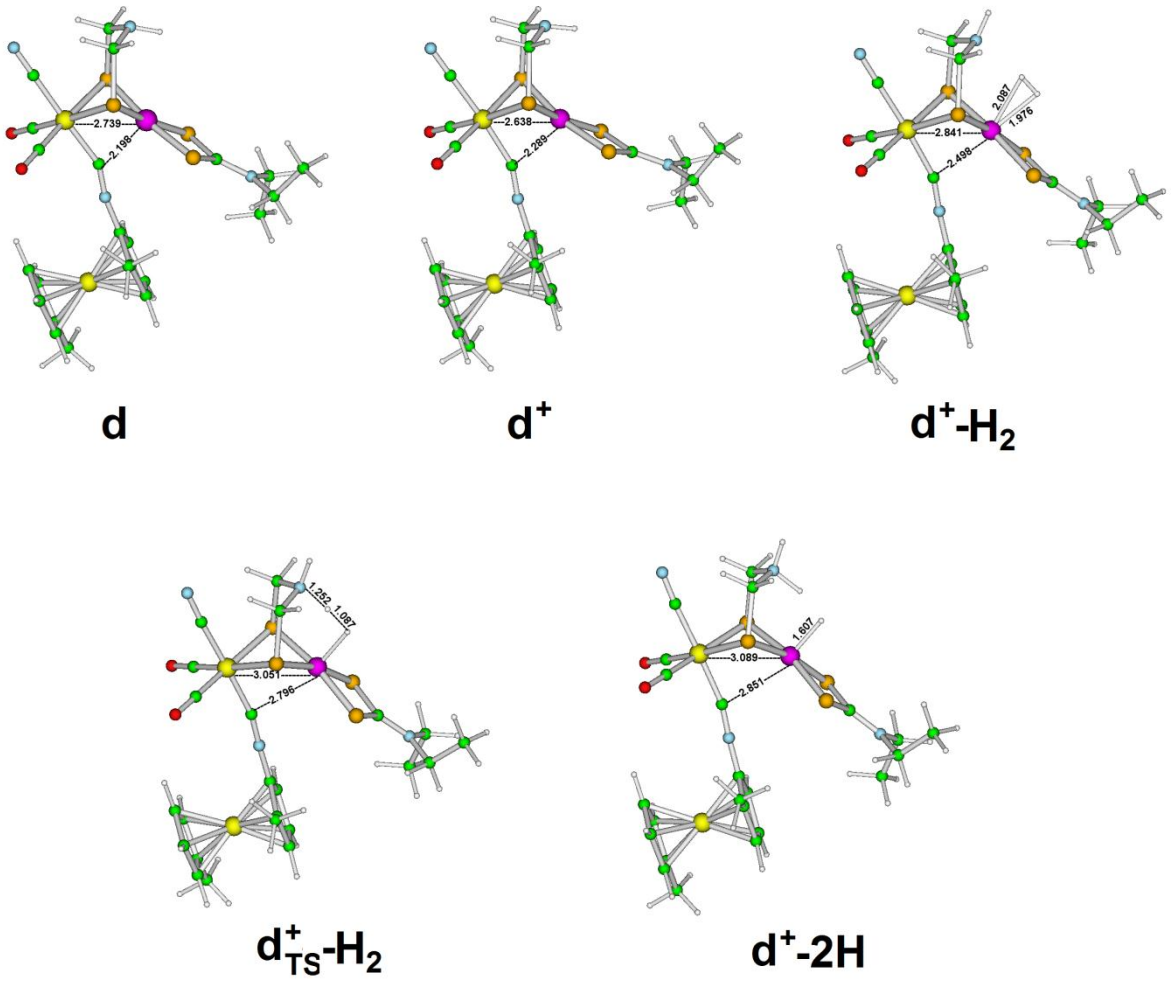


Figure S3. Ball-and-stick representation of models **d**, $\mathbf{d}^+$, $\mathbf{d}^+$**-H$_2$**, $\mathbf{d_{TS}}^+$**-H$_2$** and $\mathbf{d}^+$**-2H**. All interatomic distances in Å. Color code of atoms is the same as in Figure 4, see main text of the paper. The triplet state of **d**, as well as the quartets of the cationic models were also optimized (structures not shown). The singlet-triplet split for **d** and the doublet-quartet split for $\mathbf{d}^+$, $\mathbf{d}^+$**-H$_2$** and $\mathbf{d}^+$**-2H** are: 14.1, 17.1, 19.3, and 19.9 kcal mol^{-1}, respectively.

1.4 – Optimized structures of the Ni-containing models **e**, $\mathbf{e}^+$ and $\mathbf{e}^+$**-2H**

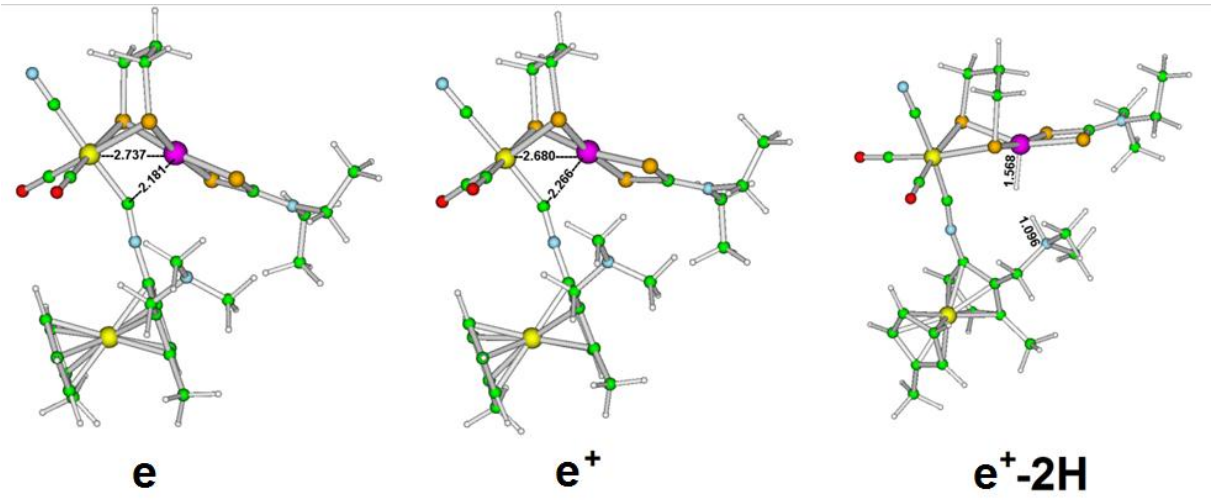


Figure S4. Ball-and-stick representation of models **e**, $\mathbf{e}^+$ and $\mathbf{e}^+$**-2H**. All interatomic distances in Å. The triplet state of **e**, as well as the quartets of the cationic models were also optimized (structures not shown). The singlet-triplet split for **e** and the doublet-quartet split for $\mathbf{e}^+$ and $\mathbf{e}^+$**-2H** are: 14.2, 17.1, 24.9 kcal mol^{-1}, respectively.

Table S1. Overall Mulliken spin populations (and charges, in parenthesis) of the mononuclear and dinuclear portions composing **c'**, $\mathbf{[c']^+}$, $\mathbf{[c']^+}$**-H_2**.

Model	Dinuclear portion	Mononuclear portion
c'	0.00 (–0.07)	0.00 (0.07)
$\mathbf{[c']^+}$	0.01 (0.07)	0.97 (0.93)
$\mathbf{[c']^+}$**-H_2**	1.01 (0.80)	–0.03 (0.20)

Table S2. Mulliken spin populations of the Ni and Fe centers in the dinuclear fragment (the latter indicated as Fe_{din}), and of the ferrocene iron atom (Fe_f) in selected Ni-containing trinuclear models.

Model	Ni	Fe_{din}	Fe_f
c	0.00	0.00	0.00
c$^+$	0.02	0.03	1.20
c$^+$**-H$_2$**	1.08	0.00	0.00
c'	0.00	0.00	0.00
[c']$^+$	0.00	0.01	1.24
[c']$^+$**-H$_2$**	1.10	0.00	–0.03
d	0.00	0.00	0.00
d$^+$	0.08	0.00	1.19
d$^+$**-H$_2$**	0.92	0.03	0.08
d$^+$**-2H**	0.63	0.01	0.01
e	0.00	0.00	0.00
e$^+$	0.16	–0.03	1.16
e$^+$**-2H**	0.72	0.00	0.00

Section 2: Results of dispersion-corrected calculations

2.1 – Optimization of model ^{disp}**b**$^-$ and comparison between experimental and computed structural and vibrational parameters

Starting from the crystal structure of **B**$^-$, we performed a geometry optimization at BP86/TZVP calculation using dispersion-corrected DFT (see Methods in the paper main text). The model thus obtained is ^{disp}**b**$^-$ (Cartesian coordinates reported below, relevant bonding interactions in Table S3). We also optimized the corresponding triplet (structure not shown), and the computed singlet-triplet splitting is found to be 10.8 kcal mol^{-1}. Such ΔE is fully consistent with the 9.8 kcal mol^{-1} singlet-triplet energy splitting reported in the paper main text for model **b**$^-$. A comparison between the computed and X-ray geometries for ^{disp}**b**$^-$ evidences a very good match (see Table S3), with most of the bond distances reproduced with deviations below 0.03 Å, and a maximum deviation of 0.06 Å for one of the Fe–S bonds. The non-bonded Fe–Ni interaction is very well reproduced (3.03 Å in ^{disp}**b**$^-$, with a deviation of 0.03 Å from crystallographic data).

Vibrational frequencies of the CN^- groups were computed, and the overall agreement with experimental values is acceptable (2110 and 2094 cm^{-1} in experiments; theoretical values at 2107 and 2122 cm^{-1}). As for the two carbonyl groups, the theoretical IR signals are located at 2014 and 1968 cm^{-1}; such frequencies are exactly the same as the one of the CO vibrational

modes in model $\mathbf{b}^-$, and can therefore be compared to experiments in an analogus way (see the paper main text). The above results show general consistency between the dispersion-corrected BP86/TZVP calculations and experiments.

Table S3. Comparison between experimental metal-to-ligand bond lengths in the Ni–Fe model $\mathbf{B}^-$ and the corresponding theoretical values in $^{disp}\mathbf{b}^-$. All values in Å.

Bond	Experimental length	Theoretical length
Ni–S	2.215, 2.198, 2.214, 2.211	2.218, 2.251, 2.259, 2.219
Fe–S	2.331, 2.343	2.393, 2.395
Fe–CO	1.783, 1.793	1.764, 1.765
Fe–CN	1.924, 1.929	1.926, 1.960

2.2 – Reactivity of model $^{disp}\mathbf{b}^-$ to dihydrogen

We then evaluated the stability of a complex between dihydrogen and $^{disp}\mathbf{b}^-$. In particular, direct coordination of H_2 with the Ni center was considered in our starting geometries for energy minimizations, in full analogy to the case of model $\mathbf{b}^-$ (see paper main text and in particular Scheme 2). Ni–H_2 coordination does not appear to correspond to any possible minimum on the singlet potential energy surface: H_2 invariably detaches along geometry optimization. In the case of the triplet, the complex turned out to be a stationary point (structure not shown), but the binding reaction is largely disfavored (+19.3 kcal mol^{-1}, a value to be compared with the 29.1 kcal mol^{-1} energy difference reported in the paper main text in the case of DFT calculations without dispersion corrections).

2.3 – Dispersion-corrected DFT calculations on models including 1-isocyano-2,1'-dimethylferrocene

The substitution of one cyanide group with 1-isocyano-2,1'-dimethylferrocene in $^{disp}\mathbf{b}^-$ gives place to model $^{disp}\mathbf{c}$ (Cartesian coordinates reported below). Optimization of models featuring the alternative disposition of isocyanide, cyanide and carbonyl groups in the Fe ion coordination sphere showed that model $^{disp}\mathbf{c}$ is the lowest minimum of the investigated potential energy surface (the disposition of ligands around metal centers in the alternative models $^{disp}\mathbf{c'}$, $^{disp}\mathbf{c}^{\S}$, $^{disp}\mathbf{c}^{\circ}$, $^{disp}\mathbf{c}^{*}$, $^{disp}\mathbf{c}^{\&}$ is the same as the one represented in Figure S1 for models $\mathbf{c'}$, $\mathbf{c}^{\S}$, $\mathbf{c}^{\circ}$, $\mathbf{c}^{*}$, $\mathbf{c}^{\&}$, respectively. See Figure S5 for details and energy differences). Therefore, in the following we will consider $^{disp}\mathbf{c}$ as our reference point for theoretical study of reactivity towards H_2. However, it has to be remarked that one of the alternative structures – the one showing the CN^- group trans to one of the carbonyl ligand, and the isocyanide coordinated trans to one of the S atom of the propanedithiolate (pdt) ligand, see model $^{disp}\mathbf{c'}$ in Figure S5 – is relatively closer in energy to $^{disp}\mathbf{c}$ (ΔE = +3.8 kcal mol^{-1}). Therefore, in the final part of the present subsection we report a detailed study on the former isomer, the reactivity of which is however similar to the one reported in the next lines for $^{disp}\mathbf{c}$.
Mulliken population analyses show that $^{disp}\mathbf{c}$ features *Fe(II)*Fe(II)Ni(II) state, see Table S4. As for the singlet-triplet energy splitting, the former state is favored by 15.8 kcal mol^{-1}, a value very close to the corresponding splitting calculated for model $\mathbf{c}$ (15.2 kcal mol^{-1}, see paper main text).

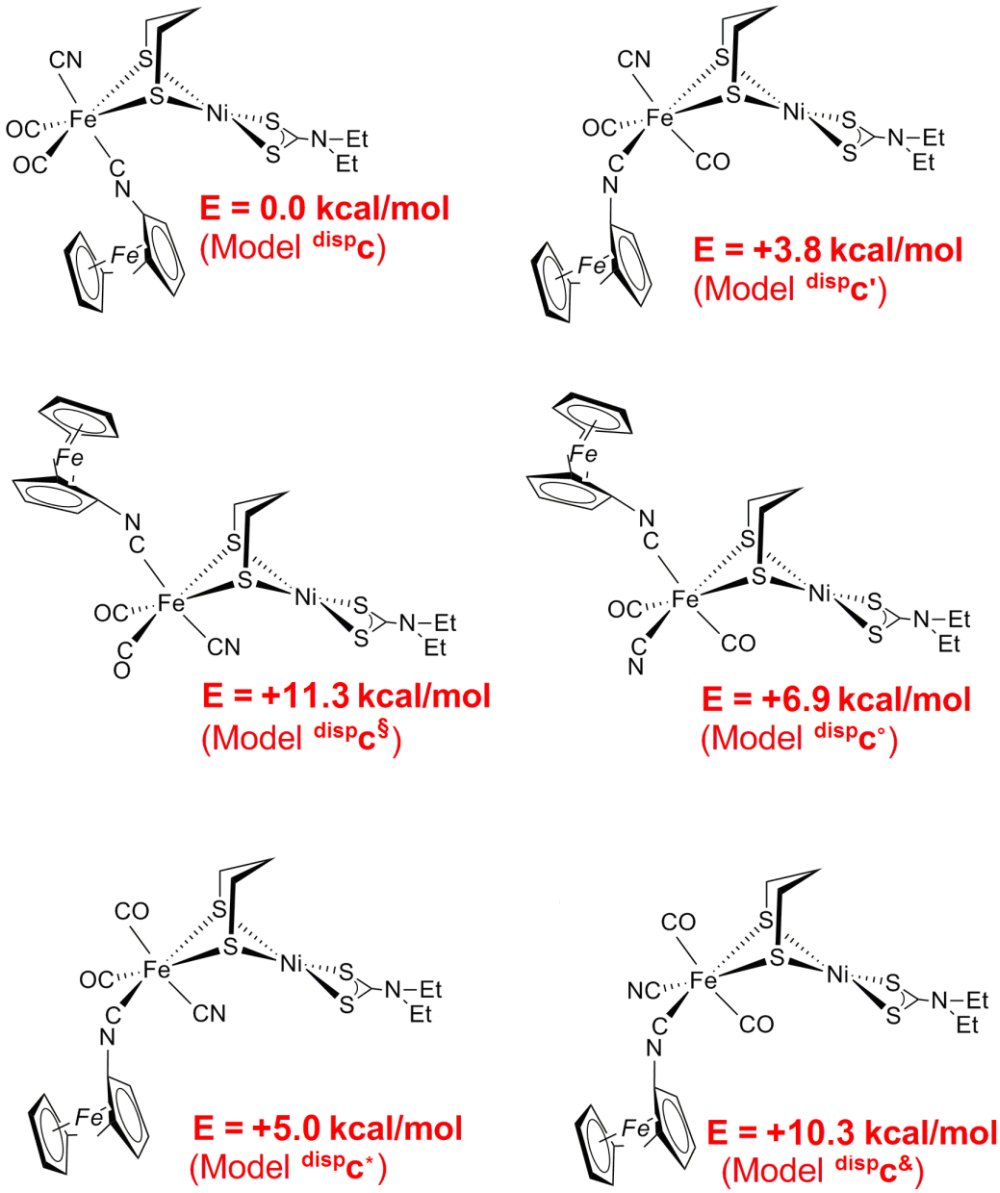


Figure S5

The one-electron oxidation of $^{disp}\mathbf{c}$ leads to $^{disp}\mathbf{c}^+$ (Cartesian coordinates of the model reported below); notably, overall spin populations and charges of the two portions composing the model indicate the *Fe(III)*Fe(II)Ni(II) state for the cationic complex. This implies that the Ni–Fe site does not change redox state, as oxidation mainly involves the metallocene fragment (see Table S4 for Mulliken charges of the two portions, and compare Table S4 with Table 3 in the paper main text to appreciate the consistency with DFT results obtained without dispersion corrections). Then, we optimized the dihydrogen complex $^{disp}\mathbf{c}^+\text{-}\mathbf{H_2}$ (Cartesian coordinates of the model reported below): analogously to model $\mathbf{c}^+\text{-}\mathbf{H_2}$ (see Figure 4 in the paper main text), the dihydrogen complex $^{disp}\mathbf{c}^+\text{-}\mathbf{H_2}$ is a minimum on the dispersion-corrected potential energy surface. Not differently from the case of H_2 binding to $\mathbf{c}^+$ (see main text), the interaction between $^{disp}\mathbf{c}^+$ and dihydrogen is associated with the oxidation of the Ni center at the expenses of the Fe ion in the metallocene sandwich. In fact, as reported in Table S4 the spin population of the dinuclear site increases from 0.07 to 0.99 going from $^{disp}\mathbf{c}^+$ to $^{disp}\mathbf{c}^+\text{-}\mathbf{H_2}$,

with the main contribution to such variation coming from the Ni ion (Mulliken spin population of Ni in $^{disp}\mathbf{c}^+$ and $^{disp}\mathbf{c}^+$-$\mathbf{H_2}$: 0.02 and 1.05, respectively, see Table S5). Concomitantly, the overall spin population of the metallocene site drops from 0.92 to zero. As far as reaction energies are concerned, H_2 attachment to the Ni center of $^{disp}\mathbf{c}^+$ is disfavored by 10.1 kcal mol^{-1} (an energy difference very close to the one computed without dispersion corrections: 10.4 kcal mol^{-1}, see paper main text); the $^{disp}\mathbf{c}^+ + H_2 \rightarrow {}^{disp}\mathbf{c}^+$-$\mathbf{H_2}$ binding reaction is characterized by a rather small barrier (10.8 kcal mol^{-1}, Cartesian coordinates of the transition state $^{disp}\mathbf{c}_{TS}{}^+$-$\mathbf{H_2}$ reported below), not differently from the results obtained for the $\mathbf{c}^+ + H_2 \rightarrow \mathbf{c}^+$-$\mathbf{H_2}$ transformation (see main text).

Finally, we analyze the reactivity of model ^{disp}**c'** (Figure S5; Cartesian coordinates below). Mulliken population analyses show that ^{disp}**c'** features the *Fe(II)*Fe(II)Ni(II) state, see Table S4. The one-electron oxidation of ^{disp}**c'** leads to ^{disp}**[c']**$^+$ (Cartesian coordinates below); notably, overall spin populations and charges of the two portions composing the model are consistent with the *Fe(III)*Fe(II)Ni(II) state for the cationic complex. This implies that the Ni–Fe site does not change redox state, in full analogy with what reported in the paper main text for the $\mathbf{c} \rightarrow \mathbf{c}^+ + e^-$ oxidation, and with the data in Table S1 for the $\mathbf{c'} \rightarrow \mathbf{[c']}^+ + e^-$ oxidation.

Then, we optimized the dihydrogen complex ^{disp}**[c']**$^+$-$\mathbf{H_2}$ (Cartesian coordinates below; the model has the same connectivity as the one of **[c']**$^+$-$\mathbf{H_2}$ in Figure S2). Most notably, H_2 binding to ^{disp}[**c'**]$^+$ is associated with the oxidation of the Ni center at the expenses of the Fe ion in the metallocene sandwich, an intramolecular redox process similar to the one observed as a result of H_2 binding to $\mathbf{c}^+$ and **[c']**$^+$ (see main text and see above). In fact – as reported in Table S4 – the spin population of the dinuclear site increases from 0.04 to 1.00 going from ^{disp}[**c'**]$^+$ to ^{disp}**[c']**$^+$-$\mathbf{H_2}$. The main contribution to such variation comes from the Ni ion (Mulliken spin population of Ni in ^{disp}**[c']**$^+$ and ^{disp}**[c']**$^+$-$\mathbf{H_2}$: 0.00 and 1.07, respectively). Concomitantly, the overall spin population of the metallocene site drops from 0.98 to –0.02. As far as reaction energies are concerned, H_2 attachment to the Ni center of ^{disp}**[c']**$^+$ is disfavored by 7.9 kcal mol^{-1} (a value comparable with the one above reported for the H_2-binding reaction on model **[c']**$^+$: 9.4 kcal mol^{-1}). Finally, the ^{disp}**[c']**$^+ + H_2 \rightarrow {}^{disp}$**[c']**$^+$-$\mathbf{H_2}$ binding reaction is characterized by a rather small barrier (8.3 kcal mol^{-1}, Cartesian coordinates of the transition state $^{disp}\mathbf{[c'}_{TS}\mathbf{]}^+$-$\mathbf{H_2}$ reported below), again analogously to the case of dihydrogen binding to **[c']**$^+$ (see above).

2.4 – Dispersion-corrected DFT calculations on models including a basic group functional for H_2 splitting

Models analogous to the **d** and **e** ones presented in the paper main text were reoptimized here using dispersion corrections. As for the first group of models, we optimized ^{disp}**d**, $^{disp}\mathbf{d}^+$, $^{disp}\mathbf{d}^+$-$\mathbf{H_2}$ and $^{disp}\mathbf{d}^+$-**2H**: the schetches in Scheme 4 (see paper main text) for models without dispersive corrections well represent also these dispersion-corrected models. Let us consider the case of model ^{disp}**d** first; computed Mulliken charges reported in Table S4 indicate that ^{disp}**d** features the *Fe(II)*Fe(II)Ni(II) state, while in the corresponding monocation $^{disp}\mathbf{d}^+$ the iron center of the metallocene is ferric. H_2 binding to the free Ni coordination site facing the dtma pendant triggers oxidation of the nickel ion at the expenses of the isocyanoferrocene (compare Mulliken populations of $^{disp}\mathbf{d}^+$-$\mathbf{H_2}$ and $^{disp}\mathbf{d}^+$ in Table S4), in full analogy to the case

of dihydrogen binding to $\mathbf{d}^+$ (see paper main text, Table 3). The $^{disp}\mathbf{d}^+ + H_2 \rightarrow {}^{disp}\mathbf{d}^+\text{-}\mathbf{H_2}$ reaction is disfavored, not differently form the case of the transformation $\mathbf{d}^+ + H_2 \rightarrow \mathbf{d}^+\text{-}\mathbf{H_2}$ presented in the paper main text; however, the difference between ΔE values is not negligible in this case: +3.5 kcal mol^{-1} in the dispersion-corrected calculation vs. the +9.8 kcal mol^{-1} energy difference reported in the main text for DFT without dispersion corrections. The path for dihydrogen splitting on $^{disp}\mathbf{d}^+\text{-}\mathbf{H_2}$ features a barrier as low as +3.5 kcal mol^{-1} (Cartesian coordinates of transition state structure $^{disp}\mathbf{d}_{TS}{}^+\text{-}\mathbf{H_2}$ reported below; notice that the barrier computed without using dispersion correction is +3.1 kcal mol^{-1}, see paper main text). The product of the $^{disp}\mathbf{d}^+\text{-}\mathbf{H_2} \rightarrow {}^{disp}\mathbf{d}^+\text{-}\mathbf{2H}$ reaction is less stable than the reactant; however, the energy difference is rather small: +2.1 kcal mol^{-1} (a value very close to the one reported in the main text for the corresponding DFT calculations without dispersion corrections: +2.9 kcal mol^{-1}).

Finally, as far as model of the **e** class are concerned, we carried out dispersion-corrected DFT optimizations of models analogous to the ones reported in Scheme 5 in the paper main text. The Cartesian coordinates of the obtained stationary points ($^{disp}\mathbf{e}^+$ and $^{disp}\mathbf{e}^+\text{-}\mathbf{2H}$) are reported below. As represented in Scheme 5, when optimization of an H_2-bound version of $^{disp}\mathbf{e}^+$ was attempted, heterolytic splitting of H_2 occurred along minimization leading to the terminal-hydride model $^{disp}\mathbf{e}^+\text{-}\mathbf{2H}$; such picture is fully consistent with the one described in the paper main test for models optimized without dispersion corrections. However, the binding reaction computed with dispersion correction is significantly more favored (ΔE = -7.3 kcal mol^{-1}) as compared to the same transformation computed without such corrections (ΔE = +0.9 kcal mol^{-1}, see paper main text).

Table S4. Overall Mulliken spin populations (and charges, in parenthesis) of the mononuclear and dinuclear portions composing each of the selected nickel-iron models

Model	Dinuclear portion	Mononuclear portion
$^{disp}\mathbf{c}$	0.00 (0.06)	0.00 (–0.06)
$^{disp}\mathbf{c}^+$	0.07 (0.28)	0.92 (0.72)
$^{disp}\mathbf{c}^+\text{-}\mathbf{H_2}$	0.99 (0.84)	0.00 (0.15)
$^{disp}\mathbf{c'}$	0.00 (–0.09)	0.00 (0.09)
$^{disp}\mathbf{[c']}^+$	0.04 (0.09)	0.98 (0.91)
$^{disp}\mathbf{[c']}^+\text{-}\mathbf{H_2}$	1.00 (0.79)	–0.02 (0.21)
$^{disp}\mathbf{d}$	0.00 (0.07)	0.00 (–0.07)
$^{disp}\mathbf{d}^+$	0.09 (0.22)	0.92 (0.78)
$^{disp}\mathbf{d}^+\text{-}\mathbf{H_2}$	0.86 (0.73)	0.09 (0.12)
$^{disp}\mathbf{d}^+\text{-}\mathbf{2H}$	0.98 (0.93)	0.02 (0.06)
$^{disp}\mathbf{e}$	0.00 (0.03)	0.00 (–0.03)
$^{disp}\mathbf{e}^+$	0.14 (0.29)	0.87 (0.71)
$^{disp}\mathbf{e}^+\text{-}\mathbf{2H}$	0.09 (0.22)	0.06 (0.78)

Table S5. Mulliken spin populations of the Ni and Fe centers in the dinuclear fragment (the latter indicated as Fe_{din}), and of the ferrocene iron atom (Fe_f) in selected Ni-containing trinuclear models.[a]

Model	Ni	Fe_{din}	Fe_f
^{disp}**c**	0.00	0.00	0.00
^{disp}**c**$^+$	0.02	0.03	1.16
^{disp}**c**$^+$**-H$_2$**	1.05	0.00	0.00
^{disp}**c'**	0.00	0.00	0.00
^{disp}**[c']**$^+$	0.00	0.04	1.20
^{disp}**[c']**$^+$**-H$_2$**	1.07	0.00	–0.03
^{disp}**d**	0.00	0.00	0.00
^{disp}**d**$^+$	0.09	0.00	1.16
^{disp}**d**$^+$**-H$_2$**	0.86	0.03	0.08
^{disp}**d**$^+$**-2H**	0.62	0.01	0.02
^{disp}**e**	0.00	0.00	0.00
^{disp}**e**$^+$	0.17	–0.03	1.12
^{disp}**e**$^+$**-2H**	0.70	0.00	0.00

[a] Notably, the reported spin populations never differ by more than 0.06 spin units from those computed in models optimized without dispersion correction (see Table S2)

Section 3: Results of calculations carried out with the COSMO continuum solvent model

In the case of calculations performed by using the COSMO continuum solvent model, vibrational frequencies cannot be computed analytically within TURBOMOLE. Therefore, vibrational spectra have not been computed in the case of COSMO-solvated models, and also the eigenvector-following approch mentioned in Methods for transition states location could not be applied. Geometry optimization of intermediates was carried out for all the models that were above considered for dispersion-corrected optimizations, while calculation of reaction barriers have been performed by simply carrying out a single point SCF calculation with COSMO at the geometry of reactants and transition states optimized in vacuo (see main text and section 1 of the supplementary information), and then using the obtained total energy values for computation of energy differences.

3.1 – Optimization of model ^{solv}**b**$^-$ and comparison between experimental and computed structural parameters

Starting from the crystal structure of **B**$^-$, we performed a geometry optimization at BP86/TZVP calculation using the COSMO continuum model for dichloromethane solvent (see Methods in the paper main text). The model thus obtained is ^{solv}**b**$^-$ (Cartesian coordinates reported below, relevant bonding interactions in Table S6). We also optimized the

corresponding triplet (structure not shown), and the computed singlet-triplet splitting is found to be 12.0 kcal mol^{-1}. Such ΔE is close to the 9.8 kcal mol^{-1} singlet-triplet energy splitting reported in the paper main text for model **b**$^{-}$. A comparison between the computed and X-ray geometries for ^{solv}**b**$^{-}$ evidences a very good match (see Table S6), with most of the bond distances reproduced with deviations below 0.03 Å, and a maximum deviation of 0.06 Å for one of the Fe–S bonds. The non-bonded Fe–Ni interaction is also reasonably well reproduced (2.97 Å in ^{disp}**b**$^{-}$, with a deviation of 0.09 Å from crystallographic data).

Table S6. Comparison between experimental metal-to-ligand bond lengths in the Ni–Fe model **B**$^{-}$ and the corresponding theoretical values in ^{solv}**b**$^{-}$. All values in Å.

Bond	Experimental length	Theoretical length
Ni–S	2.215, 2.198, 2.214, 2.211	2.221, 2.255, 2.257, 2.220
Fe–S	2.331, 2.343	2.386, 2.387
Fe–CO	1.783, 1.793	1.765, 1.765
Fe–CN	1.924, 1.929	1.924, 1.959

3.2 – Reactivity of model ^{solv}**b**$^{-}$ to dihydrogen

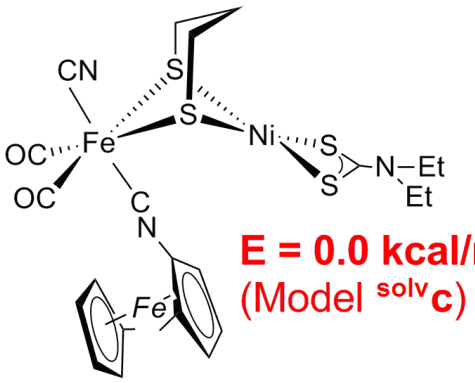
We then evaluated the stability of a complex between dihydrogen and ^{solv}**b**$^{-}$. In particular, direct coordination of H_2 with the Ni center was considered in our starting geometries for energy minimizations, in full analogy to the case of model **b**$^{-}$ (see paper main text and in particular Scheme 2). Ni–H_2 coordination does not appear to correspond to any possible minimum on the singlet potential energy surface: H_2 invariably detaches along geometry optimization. In the case of the triplet, the complex turned out to be a stationary point (structure not shown), but the binding reaction is largely disfavored (+23.6 kcal mol^{-1}, a value to be compared with the 29.1 kcal mol^{-1} energy difference reported in the paper main text in the case of DFT calculations without continuum solvent model).

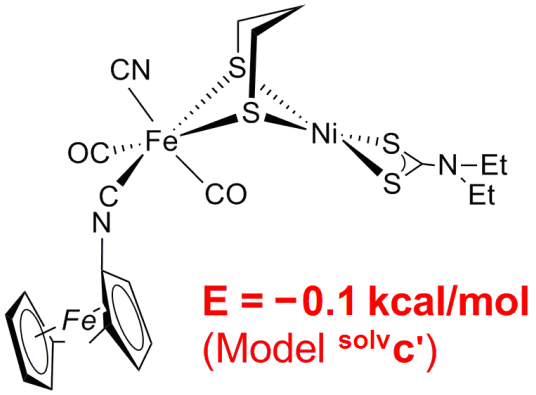
3.3 – COSMO-soaked DFT optimizations on models including 1-isocyano-2,1'-dimethylferrocene

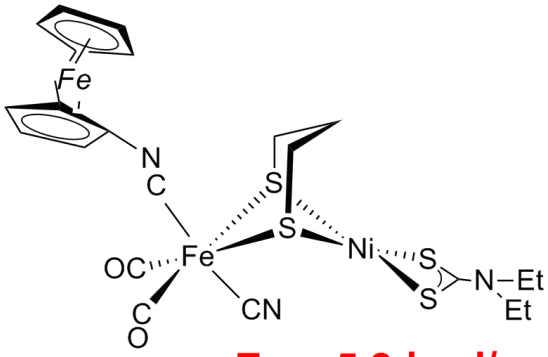
The substitution of one cyanide group with 1-isocyano-2,1'-dimethylferrocene in ^{solv}**b**$^{-}$ gives place to model ^{solv}**c** (Cartesian coordinates reported below). Optimization of models featuring the alternative disposition of isocyanide, cyanide and carbonyl groups in the Fe ion coordination sphere showed that model ^{solv}**c** and ^{solv}**c'** are significantly more stable than all the other models, while the energy difference between them is very small (0.1 kcal mol^{-1}), in full analogy with what reported in the paper main text for models **c** and **c'**, optimized *in vacuo* (the disposition of ligands around metal centers in the alternative models ^{solv}**c'**, ^{solv}**c**§, ^{solv}**c**$^{\circ}$, ^{solv}**c***, ^{solv}**c**$^{\&}$ is the same as the one represented in Figure S1 for models **c'**, **c**§, **c**$^{\circ}$, **c***, **c**$^{\&}$, respectively. See Figure S6 for details and energy differences). In the next lines we will discuss calculations on the reactivity of ^{solv}**c**, while later in this subsection we will also consider model ^{solv}**c'** in more details.
Mulliken population analyses show that ^{solv}**c** features *Fe(II)*Fe(II)Ni(II) state, see Table S7. As for the singlet-triplet energy splitting, the former state is favored by 15.4 kcal mol^{-1}, a value very close to the corresponding splitting calculated for model **c** (15.2 kcal mol^{-1}, see paper main text).

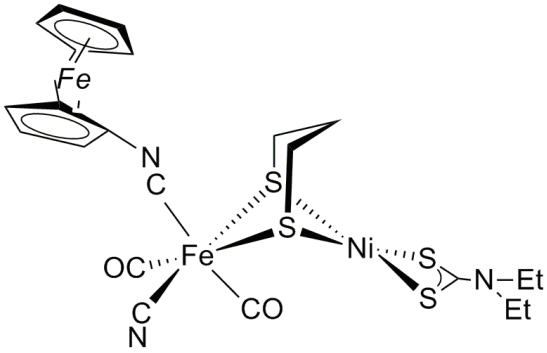
Table S7. Overall Mulliken spin populations (and charges, in parenthesis) of the mononuclear and dinuclear portions composing each of the selected nickel-iron COSMO-soaked models.

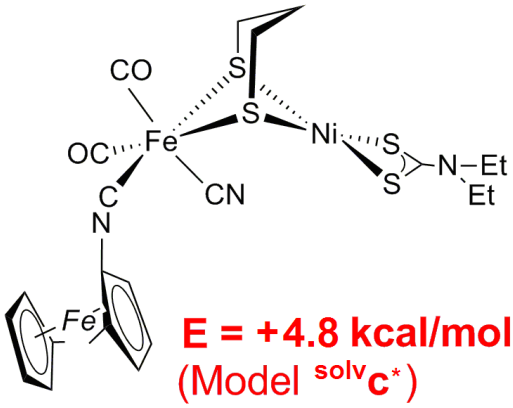
Model	Dinuclear portion	Mononuclear portion
^{solv}**c**	0.00 (–0.05)	0.00 (0.05)
^{solv}**c**$^{+}$	0.00 (0.12)	0.98 (0.88)
^{solv}**c**$^{+}$**-H$_2$**	0.98 (0.87)	0.00 (0.13)
^{solv}**c'**	0.00 (–0.10)	0.00 (0.10)
^{solv}**[c']**$^{+}$	0.01 (0.01)	0.99 (0.99)
^{solv}**[c']**$^{+}$**-H$_2$**	0.99 (0.85)	0.00 (0.15)
^{solv}**d**	0.00 (–0.06)	0.00 (0.06)
^{solv}**d**$^{+}$	0.00 (0.00)	0.98 (1.00)
^{solv}**d**$^{+}$**-2H**	1.01 (0.87)	0.01 (0.13)
^{solv}**e**	0.00 (–0.04)	0.00 (0.04)
^{solv}**e**$^{+}$	0.03 (0.12)	0.97 (0.88)
^{solv}**e**$^{+}$**-2H**	0.91 (0.14)	0.06 (0.86)


CN
S
S
OC
Fe
Ni
S
N–Et
OC
C
S
Et
N
Fe
E = 0.0 kcal/mol
(Model solvc)


CN
S
S
OC
Fe
Ni
S
N–Et
C
CO
S
Et
N
Fe
E = −0.1 kcal/mol
(Model solvc')


Fe
N
C
S
S
OC
Fe
Ni
S
N–Et
C
CN
S
Et
O
E = +5.2 kcal/mol
(Model solvc§)


Fe
N
C
S
S
OC
Fe
Ni
S
N–Et
C
CO
S
Et
N
E = +1.5 kcal/mol
(Model solvc°)


CO
S
S
OC
Fe
Ni
S
N–Et
C
CN
S
Et
N
Fe
E = +4.8 kcal/mol
(Model solvc*)

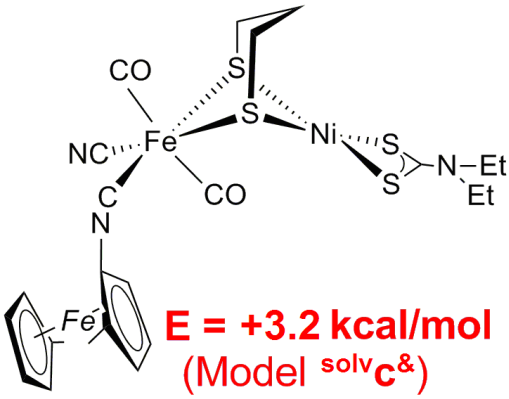

CO
S
S
NC
Fe
Ni
S
N–Et
C
CO
S
Et
N
Fe
E = +3.2 kcal/mol
(Model solvc&)

Figure S6

Table S8. Mulliken spin populations of the Ni and Fe centers in the dinuclear fragment (the latter indicated as Fe_{din}), and of the ferrocene iron atom (Fe_f) in selected Ni-containing COSMO-soaked trinuclear models.[a]

Model	Ni	Fe_{din}	Fe_f
^{solv}**c**	0.00	0.00	0.00
^{solv}**c**$^+$	0.00	0.00	1.27
^{solv}**c**$^+$**-H$_2$**	1.07	0.00	0.00
^{solv}**c'**	0.00	0.00	0.00
^{solv}**[c']**$^+$	0.00	0.01	1.25
^{solv}**[c']**$^+$**-H$_2$**	1.09	0.00	0.00
^{solv}**d**	0.00	0.00	0.00
^{solv}**d**$^+$	0.00	0.00	1.26
^{solv}**d**$^+$**-2H**	0.58	0.01	0.01
^{solv}**e**	0.00	0.00	0.00
^{solv}**e**$^+$	0.04	–0.01	1.25
^{solv}**e**$^+$**-2H**	0.68	0.00	0.00

[a] Notably, the reported spin populations never differ by more than 0.12 spin units from those computed in models optimized without inclusion of a continuum solvent model (see Table S2)

The one-electron oxidation of ^{solv}**c** leads to ^{solv}**c**$^+$ (Cartesian coordinates of the model reported below); notably, overall spin populations and charges of the two portions composing the model indicate the *Fe(III)*Fe(II)Ni(II) state for the cationic complex. This implies that the Ni–Fe site does not change redox state, as oxidation mainly involves the metallocene fragment (see Table S7 for Mulliken charges of the two portions, and compare Table S7 with Table 3 in the paper main text to appreciate the consistency with DFT results obtained without COSMO-soaking). Then, we optimized the dihydrogen complex ^{solv}**c**$^+$**-H$_2$** (Cartesian coordinates of the model reported below): analogously to model **c**$^+$**-H$_2$** (see Figure 4 in the paper main text), the dihydrogen complex ^{solv}**c**$^+$**-H$_2$** is a minimum on the potential energy surface. Not differently from the case of H_2 binding to **c**$^+$ (see main text), the interaction between ^{solv}**c**$^+$ and dihydrogen is associated with the oxidation of the Ni center at the expenses of the Fe ion in the metallocene sandwich. In fact, as reported in Table S7 the spin population of the dinuclear site increases from zero to 0.98 going from ^{solv}**c**$^+$ to ^{solv}**c**$^+$**-H$_2$**, with the main contribution to such variation coming from the Ni ion (Mulliken spin population of Ni in ^{solv}**c**$^+$ and ^{solv}**c**$^+$**-H$_2$**: 0.00 and 1.07, respectively, see Table S8). Concomitantly, the overall spin population of the metallocene site drops from 0.98 to zero. As far as reaction energies are concerned, H_2 attachment to the Ni center of ^{solv}**c**$^+$ is disfavored by 12.4 kcal mol^{-1} (an energy difference very close to the one computed for *in vacuo* optimized models: 10.4 kcal mol^{-1}, see paper main text); the ^{solv}**c**$^+$ + H_2 → ^{solv}**c**$^+$**-H$_2$** binding reaction is characterized by a rather small barrier, lower than13 kcal mol^{-1} not differently from the results obtained for the **c**$^+$ + H_2 → **c**$^+$**-H$_2$** transformation (see main text).

Finally, we analyze the reactivity of model ^{solv}**c'** (Figure S6; Cartesian coordinates below). Mulliken population analyses show that ^{solv}**c'** features the *Fe(II)*Fe(II)Ni(II) state, see Table S7. The one-electron oxidation of ^{solv}**c'** leads to ^{solv}**[c']**$^+$ (Cartesian coordinates below); notably, overall spin populations and charges of the two portions composing the model are consistent with the *Fe(III)*Fe(II)Ni(II) state for the cationic complex. This implies that the Ni–Fe site does not change redox state, in full analogy with what reported in the paper main text for the **c** → **c**$^+$ + e$^-$ oxidation, and with the data in Table S1 for the **c'** → **[c']**$^+$ + e$^-$ oxidation.

Then, we optimized the dihydrogen complex ^{solv}**[c']**$^+$**-H$_2$** (Cartesian coordinates below; the model has the same connectivity as the one of **[c']**$^+$**-H$_2$** in Figure S2). Most notably, H_2 binding to ^{solv}[**c'**]$^+$ is associated with the oxidation of the Ni center at the expenses of the Fe ion in the metallocene sandwich, an intramolecular redox process similar to the one observed as a result of H_2 binding to **c**$^+$ and **[c']**$^+$ (see main text and see above). In fact – as reported in Table S7 – the spin population of the dinuclear site increases from 0.01 to 0.99 going from ^{solv}[**c'**]$^+$ to ^{solv}**[c']**$^+$**-H$_2$**. The main contribution to such variation comes from the Ni ion (Mulliken spin population of Ni in ^{solv}**[c']**$^+$ and ^{solv}**[c']**$^+$**-H$_2$**: 0.00 and 1.09, respectively). Concomitantly, the overall spin population of the metallocene site drops from 0.99 to zero. As far as reaction energies are concerned, H_2 attachment to the Ni center of ^{solv}**[c']**$^+$ is disfavored by 11.9 kcal mol^{-1} (a value comparable with the one above reported for the H_2-binding reaction on model **[c']**$^+$: 9.4 kcal mol^{-1}). Finally, the ^{solv}**[c']**$^+$ + H_2 → ^{solv}**[c']**$^+$**-H$_2$** binding reaction is characterized by a relatively small barrier (12.6 kcal mol^{-1}), again analogously to the case of dihydrogen binding to **[c']**$^+$ (see above).

3.4 – COSMO-soaked DFT optimizations on models including a basic group functional for H_2 splitting

Models analogous to the **d** and **e** ones presented in the paper main text were reoptimized here using the COSMO continuum solvent model. As for the first group of models, we optimized ^{solv}**d**, ^{solv}**d**$^+$, and ^{solv}**d**$^+$**-2H**: the schetches in Scheme 4 (see paper main text) for models without COSMO solvation well represent also the solvated models. Let us consider the case of model ^{solv}**d** first; computed Mulliken charges reported in Table S7 indicate that ^{solv}**d** features the *Fe(II)*Fe(II)Ni(II) state, while in the corresponding monocation ^{solv}**d**$^+$ the iron center of the metallocene is ferric. As mentioned in a footnote of paper main text, **d**$^+$**-H$_2$** was among the models that were re-optimized using dispersion correction or the COSMO continuum solvent model, as reported in Methods. While the dispersion-corrected re-optimization of **d**$^+$**-H$_2$** leads to retention of H_2 binding to Ni, the same does not hold true for the COSMO re-optimization. In fact, the dihydrogen complex is not a minimum in the latter case, as H_2 detaches from the Ni ion. However, it is worth noticing that the isomer coming from H_2 splitting on the complex is a minimum also when the COSMO model is applied (^{solv}**d**$^+$**-2H**, Cartesian coordinates reported below). The reaction leading to the formation of the latter – ^{solv}**d**$^+$ + H_2 → ^{solv}**d**$^+$**-2H** – is associated wit a ΔE = +10.3 kcal mol^{-1}, which is similar to the energy difference associated to the corresponding reaction taking place *in vacuo*: ΔE = (9.8 + 2.9) kcal mol^{-1} = 12.7 kcal mol^{-1}, see main text.

Finally, as far as model of the **e** class are concerned, we carried out COSMO-soaked DFT optimizations of models analogous to the ones reported in Scheme 5 in the paper main text.

The Cartesian coordinates of the obtained stationary points (^{solv}**e**$^{+}$ and ^{solv}**e**$^{+}$**-2H**) are reported below. In fulla analogy with what represented in Scheme 5, when optimization of an H_2-bound version of ^{solv}**e**$^{+}$ was attempted, heterolytic splitting of H_2 occurred along minimization leading to the terminal-hydride model ^{solv}**e**$^{+}$**-2H**; such picture is fully consistent with the one described in the paper main text for models optimized without continuum solvent model. Finally, the energy difference associated with H_2 binding, computed using the COSMO solvent model, is similar (ΔE = –1.8 kcal mol^{-1}) to the one computed *in vacuo* (ΔE = +0.9 kcal mol^{-1}, see paper main text).

Section 4: Cartesian coordinates of models

Model **b**$^{-}$**:**

C	7.8201136	1.7664327	0.6947944
C	9.2210371	2.3294046	0.9218234
C	9.3200140	3.8531573	0.9087881
S	8.3539117	4.7064998	2.2490601
Fe	6.0541109	4.5322510	1.6336556
C	5.6180733	4.6335398	3.5466046
N	5.1934656	4.8091116	4.6304432
Ni	7.7119537	3.1316348	3.6720637
S	7.1321340	1.6208207	5.2629025
C	8.0216228	2.6447511	6.3364730
N	8.0302760	2.5124102	7.6830555
C	8.7747882	3.4511338	8.5291532
C	10.1934993	2.9703537	8.8491067
S	6.5742178	2.2307247	1.9943462
S	8.8493608	3.8970866	5.4762308
C	6.4787395	4.4297130	-0.2463655
N	6.7223633	4.3796760	-1.3964411
C	4.3670637	4.1643487	1.2821386
O	3.2576131	3.9198331	1.0419184
C	5.8828582	6.2825259	1.5143394
O	5.7715086	7.4353311	1.4302095
C	7.2092440	1.4895447	8.3424350
C	5.8072265	1.9930019	8.6981583
H	8.9713528	4.2647226	-0.0480849
H	10.3630334	4.1597705	1.0766607
H	9.6121956	1.9495214	1.8805897
H	9.8773500	1.9400035	0.1196927
H	7.8525466	0.6670882	0.7176481
H	7.4129571	2.0958604	-0.2706200
H	7.1405923	0.6304484	7.6599615
H	7.7518576	1.1565956	9.2418242
H	5.2283919	1.1907345	9.1806267
H	5.8486761	2.8466315	9.3906781
H	5.2776626	2.3099994	7.7900973
H	8.8089087	4.4151786	8.0008329
H	8.1937259	3.5987635	9.4531422
H	10.7061180	3.6999546	9.4944974
H	10.1837784	2.0018563	9.3711274
H	10.7740291	2.8621909	7.9231373

Model $[c']^{+}$-H_2:

C	0.1571474	7.5962739	-0.1639583
C	0.7678266	6.6760869	0.7486239
C	-0.2460999	5.8205250	1.2929004
C	-1.4883508	6.2027811	0.6849183
C	-1.2475998	7.3038429	-0.2022351
Fe	-0.1667495	5.6732060	-0.8386048
C	1.2774255	4.6290421	-2.0019388
C	0.2963899	3.7169961	-1.4688391
C	-1.0203841	4.1145313	-1.8984940
C	-0.8526212	5.2626299	-2.7345725
C	0.5464264	5.5802668	-2.7860985
N	0.5690225	2.6240510	-0.6925198
C	0.6105683	1.6307007	-0.0535561
Fe	0.5696911	0.1048941	0.9685083
C	1.2510582	0.7999647	2.4753773
O	1.6635580	1.2298699	3.4605282
C	2.7604924	4.5310600	-1.8388664
C	-0.0567861	4.7495138	2.3180275
C	-1.0969140	0.8811484	1.5575376
N	-2.0643440	1.4583312	1.8865028
C	2.2168928	-0.3735149	0.3871601
O	3.3073266	-0.5252661	0.0405395
Ni	0.2119677	-3.1314151	0.0901569
S	-0.5187119	-1.1508889	-0.7362140
C	-2.2902351	-1.3250978	-0.1745960
C	-2.5033633	-2.2852194	0.9974434
C	-1.7009713	-2.0283294	2.2733160
S	0.1473901	-1.9663346	2.0300018
S	-0.2277470	-4.4419287	-1.7162173
C	0.0497127	-5.7886699	-0.6432505
S	0.4168403	-5.2228087	0.9643989
N	-0.0101163	-7.0680039	-1.0009732
C	-0.3358656	-7.4653453	-2.3879876
C	-1.8261505	-7.7408241	-2.5905803
C	0.2500581	-8.1517318	-0.0277989
C	1.7085092	-8.6119485	-0.0322044
H	-2.6490545	-0.3139163	0.0483708
H	-2.8134584	-1.7083520	-1.0614901
H	-2.3084742	-3.3157699	0.6551657
H	-3.5737471	-2.2456007	1.2656260
H	-1.8507481	-2.8601525	2.9752177
H	-1.9850084	-1.0902529	2.7641374
H	-0.0415793	-7.7858104	0.9662856
H	-0.4276599	-8.9781601	-0.2852145
H	1.8361419	-9.4293533	0.6907279
H	2.0142151	-8.9866636	-1.0188895
H	2.3798478	-7.7924995	0.2559247
H	0.0080859	-6.6622406	-3.0544413
H	0.2657407	-8.3580992	-2.6108548
H	-2.0023662	-8.0545290	-3.6287311
H	-2.1851494	-8.5442392	-1.9324125
H	-2.4219517	-6.8387013	-2.4000865
H	3.2363609	5.5151152	-1.9326643
H	3.0368509	4.1012967	-0.8671285
H	3.1834477	3.8809974	-2.6217744
H	0.9631833	4.3434387	2.2951915
H	-0.2156044	5.1727903	3.3232677
H	-0.7742975	3.9268231	2.1930257
H	-1.9456696	3.6070552	-1.6424362
H	-1.6501223	5.8026067	-3.2367129
H	0.9918833	6.4089180	-3.3304625
H	1.8277719	6.6240973	0.9867377
H	0.6661836	8.3721233	-0.7292508
H	-1.9936812	7.8194794	-0.8006226
H	-2.4480419	5.7256199	0.8682367
H	2.2161304	-3.1887347	0.0266177
H	2.0531622	-2.9708314	-0.6945681

Model $[c']_{TS}^{+}$-H_2:

C	9.4841911	1.5763987	-4.8068053
C	9.5074900	0.3718248	-4.0357200
C	8.2966968	0.3799022	-3.2517735
C	7.5479067	1.5828290	-3.5248328
C	8.2900495	2.3117926	-4.5071457
Fe	9.4068604	2.0965981	-2.7845226
C	10.2358006	3.9403731	-2.3484920
C	11.2234393	2.9060736	-2.2351079
C	10.7847207	1.9953383	-1.2183419
C	9.5370538	2.4650334	-0.6851900
C	9.1991889	3.6597713	-1.4011837
C	8.7497220	1.8429042	0.4233702
C	10.5237862	-0.7223575	-4.0836388
N	7.8957050	-0.6206433	-2.4098355
C	7.3474229	-1.4149607	-1.7273732
Fe	6.4093463	-2.6014336	-0.6899167
S	4.8887550	-4.1326414	0.2882183
C	3.1930349	-3.4870723	-0.1480774
C	2.7892266	-3.6984221	-1.6084278
C	3.7155583	-3.1302207	-2.6858218
S	5.4868124	-3.7102602	-2.5847957
Ni	5.0785692	-5.6012571	-1.4165368
S	4.2344851	-7.4376585	-0.3866019
C	4.2475376	-8.1690081	-1.9697603
N	3.8266559	-9.4005364	-2.2413490
C	3.2920619	-10.2862989	-1.1833146
C	4.3501121	-11.2259789	-0.6052571
C	6.8246426	-1.9089429	0.9132333
O	7.0657580	-1.4668756	1.9488343
C	5.0982553	-1.1872869	-0.7782648
N	4.3879622	-0.2558851	-0.8474649
C	7.8342340	-3.7171944	-0.6339639
O	8.8427497	-4.2769438	-0.5825574
S	4.8813469	-7.0525839	-3.1505786
C	3.8613613	-9.9360437	-3.6198033
C	2.5557644	-9.6994914	-4.3805696
H	3.7438764	-2.0348692	-2.6711262
H	3.3798533	-3.4708232	-3.6747277
H	2.6496104	-4.7783334	-1.7873373
H	1.7980385	-3.2316274	-1.7478342
H	2.5150682	-4.0513245	0.5068259
H	3.1735431	-2.4302554	0.1411490
H	2.8649436	-9.6477112	-0.3981120
H	2.4632770	-10.8515321	-1.6334099
H	3.8887439	-11.8720722	0.1544603
H	4.7844429	-11.8757453	-1.3776070
H	5.1600466	-10.6601961	-0.1268048
H	4.7075514	-9.4653433	-4.1393392
H	4.0823932	-11.0093637	-3.5363346
H	2.6331598	-10.1385147	-5.3846689
H	1.6995333	-10.1672184	-3.8751021
H	2.3549845	-8.6257996	-4.4910910
H	11.5101856	-0.3377863	-4.3715265
H	10.6156235	-1.2369453	-3.1182955
H	10.2290772	-1.4740718	-4.8336829
H	8.9111168	0.7585827	0.4766852
H	9.0701467	2.2676190	1.3883906
H	7.6740547	2.0350507	0.3193901
H	6.5889033	1.8407914	-3.0842094
H	8.0012967	3.2650051	-4.9410735
H	10.2634530	1.8858258	-5.4988142
H	11.3057772	1.0954876	-0.8992096
H	12.1366316	2.8250371	-2.8182774
H	10.2627924	4.7797289	-3.0381371
H	8.2919221	4.2417168	-1.2577597
H	7.0705893	-6.4748375	-0.7187692
H	7.1506947	-6.4173152	-1.4731177

Model **[c']$^+$:**

O	7.2444672	-4.9059736	-1.3843276
C	4.6487684	-0.8866344	-0.4552163
Fe	5.4455374	-2.6046428	-0.7979999
C	6.5914833	-1.6135943	-1.8331408
N	7.2931304	-0.9140874	-2.4758877
C	6.3618522	-4.1752382	-1.2012727
Ni	4.2032603	-4.8334287	-1.4621904
S	4.3876271	-6.2199186	-3.2161354
C	4.4771885	-7.5007102	-2.0306560
N	4.5964811	-8.7928638	-2.3121446
C	4.6834201	-9.8072924	-1.2375397
C	6.1268657	-10.1482600	-0.8652906
N	4.2042132	0.1847896	-0.2815054
S	4.3602963	-6.8323581	-0.4270580
S	3.7447063	-3.7068889	0.4137103
C	2.1709876	-2.7473923	0.1955754
C	1.5539197	-2.8108462	-1.1969902
C	2.3825995	-2.1479094	-2.2916285
S	4.0149728	-2.9527689	-2.6593316
C	4.6450544	-9.2764029	-3.7098895
C	3.2722877	-9.6983158	-4.2357870
C	6.3584771	-2.4154898	0.7357822
O	6.9277063	-2.2723734	1.7257805
H	2.6021409	-1.0989153	-2.0492244
H	1.8529554	-2.1906266	-3.2530853
H	1.3340453	-3.8558190	-1.4672809
H	0.5850146	-2.2843330	-1.1524731
H	1.4960071	-3.1970159	0.9365903
H	2.3899340	-1.7130080	0.4937767
H	4.1340897	-9.4209610	-0.3678055
H	4.1454136	-10.6960556	-1.5964638
H	6.1292752	-10.9184846	-0.0816254
H	6.6863875	-10.5431082	-1.7245941
H	6.6526642	-9.2652486	-0.4792343
H	5.0709864	-8.4725885	-4.3259093
H	5.3533791	-10.1167774	-3.7303397
H	3.3739928	-10.0712155	-5.2642560
H	2.8332207	-10.5029456	-3.6298223
H	2.5771453	-8.8485684	-4.2462680
C	7.8955813	0.0508494	-3.2373179
C	7.4929293	1.4351930	-3.2884549
C	8.3316562	2.0701457	-4.2569057
C	9.2503418	1.0945155	-4.7668199
C	8.9988335	-0.1682995	-4.1409145
Fe	9.4760446	1.3242056	-2.7064664
C	9.6659366	-1.4746867	-4.4268658
H	10.6966133	-1.3271930	-4.7735259
H	9.6854476	-2.1250748	-3.5428923
H	9.1209585	-2.0086894	-5.2217311
C	10.7598357	0.6396519	-1.2289625
C	9.7980500	1.5191267	-0.6177053
C	9.9259140	2.7910293	-1.2651272
C	10.9617733	2.7087664	-2.2478053
C	11.4839999	1.3744070	-2.2258335
C	8.8751695	1.1850806	0.5115880
H	8.6107855	0.1204402	0.5184168
H	9.3698113	1.4046744	1.4714692
H	7.9512044	1.7754844	0.4738516
H	6.6806671	1.8755064	-2.7170003
H	8.2865545	3.1172644	-4.5447129
H	10.0322135	1.2786068	-5.4999377
H	10.9140193	-0.4041443	-0.9661134
H	12.2785128	0.9878898	-2.8587178
H	11.2776848	3.5098976	-2.9110329
H	9.3106939	3.6641788	-1.0608506

Model **c':**

O	7.0534812	-4.5484756	-1.0785257
C	4.1782769	-0.7007040	-0.1742127
Fe	5.1400683	-2.3298552	-0.5457078
C	6.2625691	-1.3385434	-1.5986712
N	6.9725257	-0.6941234	-2.2880498
C	6.1036303	-3.8822994	-0.9449604
Ni	4.0963674	-4.6728539	-1.3509107
S	4.5735910	-5.9130309	-3.1759622
C	4.6738353	-7.2523041	-2.0752294
N	4.9518180	-8.5143360	-2.4314779
C	5.0290127	-9.5907790	-1.4281242
C	6.4515289	-9.8213434	-0.9134567
N	3.5979041	0.2968903	0.0418256
S	4.3426501	-6.7294369	-0.4531850
S	3.5022920	-3.6625349	0.5519335
C	1.8644488	-2.8140419	0.3500761
C	1.2753709	-2.8641539	-1.0549618
C	2.0732380	-2.0913010	-2.0987191
S	3.7637497	-2.7644653	-2.4630509
C	5.1974848	-8.8714637	-3.8392936
C	3.9332234	-9.3357537	-4.5660763
C	6.0308479	-2.0828963	0.9633461
O	6.6038276	-1.9046971	1.9528753
H	2.2105755	-1.0441610	-1.7956281
H	1.5614338	-2.1221900	-3.0707564
H	1.1528476	-3.9120943	-1.3743958
H	0.2648569	-2.4195453	-1.0097959
H	1.2076520	-3.3376840	1.0587521
H	2.0027217	-1.7768402	0.6850814
H	4.3570979	-9.3238474	-0.6003045
H	4.6263638	-10.5010894	-1.8967296
H	6.4543366	-10.6419125	-0.1816381
H	7.1380690	-10.0940984	-1.7276377
H	6.8355123	-8.9187088	-0.4207726
H	5.6260047	-7.9897364	-4.3362831
H	5.9666510	-9.6584219	-3.8450943
H	4.1770665	-9.6048191	-5.6037610
H	3.4902420	-10.2187130	-4.0838618
H	3.1821814	-8.5348242	-4.5867364
C	7.7153779	0.0799254	-3.1391608
C	7.5938793	1.5090542	-3.2933314
C	8.4953781	1.8926395	-4.3355233
C	9.1722849	0.7180816	-4.8049322
C	8.7109061	-0.4224874	-4.0662713
Fe	9.5177152	0.9916675	-2.7925031
C	9.0770457	-1.8577288	-4.2769028
H	10.0984942	-1.9487818	-4.6703405
H	9.0150287	-2.4323686	-3.3435381
H	8.3948820	-2.3309873	-5.0025826
C	10.5823250	0.1104789	-1.2616596
C	9.8787836	1.2636475	-0.7641117
C	10.3418445	2.3946789	-1.5217556
C	11.3175932	1.9457821	-2.4709415
C	11.4674413	0.5285610	-2.3087296
C	8.8996730	1.2901726	0.3689608
H	8.3309697	0.3535989	0.4352256
H	9.4244752	1.4240774	1.3292201
H	8.1836309	2.1163933	0.2643326
H	6.9250865	2.1476647	-2.7242194
H	8.6580088	2.9071336	-4.6891785
H	9.9374743	0.6912463	-5.5772098
H	10.4448120	-0.9101907	-0.9116610
H	12.1184038	-0.1163802	-2.8932952
H	11.8319794	2.5641676	-3.2021226
H	9.9844537	3.4156409	-1.4092494

Model **c**:

C	3.5598478	4.7315471	3.7515526
C	3.8114984	5.0960986	5.1129808
C	5.0860429	5.7537715	5.1768097
C	5.6542620	5.8162924	3.8594114
C	4.7099461	5.1489310	2.9818079
Fe	3.8157601	6.7589531	3.9137789
C	2.0962966	7.6514244	3.2030738
C	3.2358425	8.1109015	2.4654316
C	4.1422403	8.7241120	3.3905178
C	3.5549526	8.6456139	4.6972771
C	2.2833214	7.9811109	4.5914775
C	1.2994472	7.7587623	5.7007731
C	7.0020888	6.3344275	3.4679482
N	4.8869100	4.9497791	1.6477781
C	5.1249449	4.6052292	0.5289367
Fe	5.1507675	4.8535639	-1.3871253
C	5.2126853	5.0519524	-3.2997796
N	5.2561349	5.1685448	-4.4671868
C	3.4526901	5.3635595	-1.4072759
O	2.3459317	5.6988109	-1.4269625
C	5.8318498	6.4804555	-1.2188002
O	6.2768965	7.5430212	-1.1128174
S	7.3357695	3.9003994	-1.3446540
Ni	6.0514673	2.6836818	0.0241364
S	7.6014948	2.4642567	1.6557524
C	6.4721690	1.3737577	2.3992597
N	6.7135799	0.6728244	3.5164662
C	5.7060434	-0.2442030	4.0758222
C	4.8410904	0.4097673	5.1545707
S	4.4975578	2.5654714	-1.5763093
C	5.2558969	1.9068487	-3.1369259
C	6.7676446	1.7104971	-3.0936242
C	7.5736599	2.9968080	-2.9481919
S	5.0108168	1.2824834	1.4654304
C	8.0064238	0.7796027	4.2151445
C	9.0240963	-0.2622801	3.7455306
H	5.5452869	6.1657259	6.0722122
H	3.1389084	4.9242817	5.9489904
H	5.1089423	9.1562222	3.1465791
H	3.9996425	9.0106604	5.6201869
H	7.3349768	3.7089872	-3.7494484
H	8.6500069	2.7755766	-2.9699222
H	7.0311105	1.0101430	-2.2844318
H	7.0688187	1.2343940	-4.0442976
H	4.7514430	0.9423635	-3.2896092
H	4.9675671	2.5961728	-3.9422243
H	5.0825248	-0.5997115	3.2434065
H	6.2456669	-1.1150957	4.4775152
H	4.1167203	-0.3195090	5.5449467
H	5.4480071	0.7673707	5.9987173
H	4.2852713	1.2615344	4.7414134
H	8.3924603	1.7954097	4.0491889
H	7.8028755	0.6768712	5.2911582
H	9.9618063	-0.1482914	4.3080810
H	8.6578179	-1.2865049	3.9044883
H	9.2453594	-0.1310775	2.6782022
H	6.9911449	6.7674160	2.4587558
H	7.3445948	7.1068267	4.1696886
H	7.7454728	5.5202444	3.4667850
H	1.2384444	7.1280204	2.7874651
H	3.3965192	7.9889896	1.3976963
H	1.8039583	7.6458208	6.6705223
H	0.6112570	8.6164595	5.7846186
H	0.6889167	6.8626261	5.5241981
H	2.6914956	4.2166489	3.3520193

Model $\mathbf{c}^{+}$:

C	3.5431982	4.9723615	3.9184015
C	3.8225933	5.3986213	5.2551949

C	5.1167352	6.0152008	5.2697664
C	5.6790624	5.9769982	3.9541963
C	4.7041407	5.3054850	3.1228275
Fe	3.8275978	7.0103711	3.9676314
C	2.2935620	7.9471989	2.9448375
C	3.5613454	8.4953329	2.5518193
C	4.1752945	9.0543683	3.7167309
C	3.2872569	8.8543616	4.8192702
C	2.1106334	8.1800002	4.3524720
C	0.8976493	7.8402297	5.1603999
C	7.0324962	6.4441584	3.5250848
N	4.8589015	5.0349491	1.7986361
C	5.0629599	4.6588656	0.6864120
Fe	5.0910327	4.7554253	-1.2220535
C	5.0888351	4.9744200	-3.1301771
N	5.0956050	5.0976130	-4.2962846
C	3.3620356	5.2364598	-1.2470561
O	2.2535862	5.5431145	-1.2719297
C	5.7769445	6.4112340	-1.1414103
O	6.2182535	7.4731274	-1.0992323
S	7.2811517	3.8787229	-1.2730242
Ni	6.0014030	2.6933892	0.1252124
S	7.6092416	2.4330252	1.6834490
C	6.5330868	1.2659952	2.4070352
N	6.8416903	0.4782253	3.4318409
C	5.8753213	-0.5071323	3.9636482
C	5.0618919	0.0361773	5.1385714
S	4.4233612	2.5024267	-1.4400814
C	5.1743198	1.8302070	-2.9968989
C	6.6881178	1.6531485	-2.9769615
C	7.4867789	2.9468520	-2.8638575
S	5.0212399	1.2351363	1.5403965
C	8.1803076	0.5263886	4.0615866
C	9.1473925	-0.4995718	3.4696295
H	5.5968738	6.4651840	6.1351961
H	3.1587159	5.2868456	6.1077435
H	5.1528019	9.5275344	3.7615063
H	3.4800914	9.1406940	5.8503975
H	7.2317597	3.6519730	-3.6668426
H	8.5647249	2.7375207	-2.8997688
H	6.9775984	0.9577564	-2.1735579
H	6.9737824	1.1746464	-3.9298449
H	4.6744396	0.8597770	-3.1223651
H	4.8557609	2.5034732	-3.8050421
H	5.2169598	-0.8082512	3.1369352
H	6.4556603	-1.3922282	4.2603758
H	4.3819129	-0.7451922	5.5046731
H	5.7075784	0.3378868	5.9749460
H	4.4568029	0.8995318	4.8316948
H	8.5710110	1.5461145	3.9391186
H	8.0312019	0.3583473	5.1374976
H	10.1148968	-0.4295509	3.9854092
H	8.7772635	-1.5267808	3.5914474
H	9.3140711	-0.3103992	2.4012637
H	7.0195835	6.8610339	2.5096139
H	7.4213373	7.2090961	4.2089120
H	7.7411068	5.6000973	3.5249241
H	1.5809959	7.4504379	2.2911950
H	3.9834048	8.4834262	1.5507708
H	1.1440359	7.6822712	6.2185058
H	0.1753641	8.6710904	5.1119464
H	0.3915821	6.9438066	4.7787620
H	2.6587431	4.4563245	3.5574209

Model $\mathbf{c_{TS}}^{+}$**-H$_2$**:

C	1.7936050	6.4268903	3.0464263
C	1.9773695	6.0931531	4.4272423
C	3.3835280	6.0016254	4.6722617
C	4.0864246	6.2672017	3.4511412
C	3.0934498	6.5443664	2.4486639
Fe	2.8669913	7.9217269	3.9810634
C	4.1055521	9.5076087	4.4996571
C	3.1420821	9.3076399	5.5386642

C	1.8244350	9.4597135	5.0049011
C	1.9944913	9.7658062	3.6001891
C	3.4059654	9.7799536	3.2825652
H	3.3665687	9.0501421	6.5710286
C	0.5292611	9.4063607	5.7498165
N	0.9836206	10.0605835	2.7271770
C	0.1368232	10.3834513	1.9631366
Fe	-1.1511070	10.6012033	0.6412812
C	0.0445576	10.1939018	-0.6339183
O	0.8112364	9.9504290	-1.4572761
H	5.1846149	9.4442461	4.6098748
H	1.1901328	5.9492475	5.1626362
H	3.8498571	5.7918600	5.6321548
C	5.5677928	6.2123690	3.2461482
C	-1.7570183	8.9389857	0.9254677
O	-2.1593396	7.8760769	1.1131947
S	-2.6928021	11.5582290	2.1709299
C	-3.9774505	12.4055602	1.1153001
C	-3.5017280	13.6962737	0.4425161
C	-2.2466824	13.6265989	-0.4316103
S	-0.7402484	12.9329726	0.4241559
Ni	-1.4194834	13.3930656	2.5249490
S	-0.5359380	15.4797098	2.7148614
C	-1.5451612	15.6327729	4.1298476
N	-1.6606365	16.7378398	4.8605095
C	-2.5700385	16.7997655	6.0262806
C	-3.9549987	17.3399804	5.6671345
C	-2.4309584	10.6292281	-0.7982155
N	-3.1921618	10.5963133	-1.6897096
S	-2.4046555	14.1449826	4.4348740
C	-0.9053228	17.9659869	4.5272238
C	0.4090903	18.0813683	5.2997229
H	-4.3238342	11.6612462	0.3897383
H	-4.7906729	12.6362231	1.8167307
H	-3.3552517	14.4697726	1.2165033
H	-4.3269011	14.0551415	-0.1973837
H	-1.9451918	14.6422717	-0.7218640
H	-2.3996971	13.0221987	-1.3327009
H	-0.7234789	17.9626132	3.4437632
H	-1.5686455	18.8145570	4.7460906
H	0.9094886	19.0221245	5.0310563
H	0.2437267	18.0886604	6.3858705
H	1.0843603	17.2520510	5.0521075
H	-2.6428023	15.7877770	6.4478054
H	-2.0792080	17.4352588	6.7769161
H	-4.5754299	17.3864313	6.5726576
H	-3.9007273	18.3532775	5.2457999
H	-4.4559314	16.6848276	4.9424416
H	0.5104139	12.8475882	3.5340662
H	0.0046508	12.5130225	3.9943520
H	-0.2906413	9.0369749	5.1201720
H	0.6068965	8.7626304	6.6349806
H	0.2518530	10.4144896	6.0984277
H	3.2996253	6.7915379	1.4100150
H	0.8410208	6.5678981	2.5425138
H	6.1158545	6.4493511	4.1674827
H	5.8608119	5.1944272	2.9426090
H	5.8958037	6.8974726	2.4536116
H	3.8336126	9.9995781	2.3088154

Model $\mathbf{c^{+}\text{-}H_2}$:

C	3.2599534	9.5567594	3.3870826
C	4.0456210	9.2577944	4.5426253
C	3.1737665	9.2156146	5.6812823
C	1.8302110	9.4980587	5.2608190
C	1.9019989	9.7266352	3.8348764
Fe	2.6056500	7.7995280	4.2868218
C	3.2239142	6.1350361	3.1606053
C	1.8193266	6.3527168	3.0129084
C	1.2210316	6.2690327	4.3134028
C	2.2683994	6.0004759	5.2562312
C	3.5152020	5.9063722	4.5460986
C	4.8508324	5.5753460	5.1349488

C	0.6167099	9.6329868	6.1243143
N	0.8424638	10.0594189	3.0380197
C	-0.0659352	10.3882726	2.3507226
Fe	-1.5313881	10.5588498	1.2160299
C	-3.0486071	10.4833232	0.0325630
N	-3.9687581	10.3822877	-0.6875273
C	-0.7016578	9.5787607	-0.0382611
O	-0.1691636	8.9661940	-0.8543132
C	-2.3535298	9.2107372	2.0666604
O	-2.8932103	8.3556854	2.6173431
S	-2.5532504	12.2090363	2.5813724
Ni	-0.9258410	13.7413847	2.2083243
S	-1.4841270	15.2311981	3.8441421
C	-0.4666132	16.3556016	2.9808570
N	-0.2817763	17.6265918	3.3248520
C	0.5998604	18.5166541	2.5369638
C	2.0321168	18.5522871	3.0716025
S	-0.7744261	12.5943871	0.2613674
C	-2.2734347	13.3494435	-0.5528238
C	-3.3077757	13.9282153	0.4153814
C	-3.8544077	13.0066280	1.5084960
S	0.2557192	15.5901627	1.5907961
C	-0.9596919	18.2128086	4.5024033
C	-2.2755409	18.9033736	4.1427934
H	3.4712779	9.0031183	6.7049485
H	5.1175257	9.0812045	4.5502900
H	0.1653534	6.3843680	4.5433328
H	2.1472823	5.8850518	6.3307217
H	-4.4611168	12.1905414	1.0997044
H	-4.4604665	13.5919820	2.2132907
H	-2.8875072	14.8324220	0.8873229
H	-4.1680450	14.2665866	-0.1880796
H	-1.8610763	14.1558823	-1.1745743
H	-2.6970429	12.5736757	-1.2005452
H	0.5796779	18.1701685	1.4945922
H	0.1427204	19.5160067	2.5602292
H	2.6309955	19.2464095	2.4661500
H	2.0687082	18.8985453	4.1136898
H	2.4976187	17.5594904	3.0143195
H	-1.1272893	17.4046680	5.2275816
H	-0.2511398	18.9206897	4.9557042
H	-2.7209200	19.3376001	5.0483736
H	-2.1238974	19.7174183	3.4206578
H	-2.9918775	18.1872737	3.7194514
H	0.7098447	12.9844943	2.8561976
H	0.2572507	12.9740447	3.4882396
H	-0.3017798	9.3747184	5.5814906
H	0.6884505	8.9883261	7.0094185
H	0.5140783	10.6709627	6.4793407
H	3.9598023	6.1666951	2.3604156
H	1.3022553	6.5629819	2.0804438
H	4.9417450	5.9365517	6.1677884
H	4.9855308	4.4819275	5.1564623
H	5.6735146	5.9952102	4.5415207
H	3.6038526	9.6559815	2.3617427

Model **d:**

C	3.6113995	4.7110964	3.8293861
C	3.7842065	5.1025737	5.2159902
C	5.0596021	5.7653990	5.3677980
C	5.6987906	5.7429804	4.0866162
C	4.8173955	5.1005454	3.1530164
Fe	3.9153604	6.7492207	3.9800104
C	3.3926905	7.9900894	2.4227898
C	4.3496215	8.6492844	3.2716778
C	3.7675678	8.7175519	4.5859217
C	2.4705005	8.1104447	4.5458243
C	2.2377219	7.6566065	3.2062064
C	5.6641855	9.2329761	2.8481774
N	2.8859920	4.8740490	6.2129937
C	2.2312152	4.4857325	7.1338506
Fe	0.8135589	4.6087777	8.4355950
C	-0.3921915	4.9760627	7.1884133

O	-1.1841011	5.2119605	6.3791814
C	2.4580038	3.9392166	3.2708251
Ni	2.6636474	2.6048736	8.1856835
S	3.1564314	1.2174107	6.4716782
C	4.8180167	1.4873924	6.9022134
N	5.8644374	0.8864511	6.3180038
C	7.2449713	1.1621512	6.7513018
C	7.9326633	2.2330983	5.9019544
S	4.9228297	2.6087066	8.2244325
S	2.4003551	3.8243398	10.0408277
C	1.4167147	2.7673358	11.2954365
N	0.9152848	1.5171546	10.8218278
C	-0.0860250	1.5692198	9.8054783
S	0.4526542	2.2703595	8.1081752
C	5.6704639	-0.0866460	5.2290339
C	5.5659767	-1.5288000	5.7301376
C	-0.5714738	4.6912376	9.7706323
N	-1.4118577	4.7378157	10.5891906
C	1.2258675	6.2926380	8.8055292
O	1.4864796	7.3924187	9.0506137
H	5.0122059	4.9497106	2.0937471
H	6.6745119	6.1635395	3.8578358
H	1.3499889	7.1394520	2.8513089
H	3.5338852	7.7683902	1.3674816
H	-0.9236640	2.1990034	10.1285131
H	-0.4306955	0.5569757	9.5643661
H	1.6676483	0.8666468	10.5861176
H	2.1348366	2.6014000	12.1067932
H	0.5912797	3.4065749	11.6309437
H	7.2062176	1.4712270	7.8052911
H	7.7961088	0.2109082	6.7079022
H	8.9592074	2.3912502	6.2627230
H	7.9896174	1.9374983	4.8445295
H	7.3916501	3.1860773	5.9669645
H	4.7584038	0.1982203	4.6857628
H	6.5161308	0.0301705	4.5353518
H	5.4397006	-2.2115142	4.8776794
H	6.4700770	-1.8346158	6.2758854
H	4.6997574	-1.6449756	6.3944236
H	1.5144650	4.2128337	3.7616642
H	2.3499526	4.1192281	2.1927123
H	2.6041133	2.8574413	3.4242093
H	4.2434640	9.1437584	5.4658642
H	1.7969789	7.9879964	5.3893519
H	6.1037904	8.6719919	2.0119725
H	5.5349059	10.2762570	2.5154141
H	6.3874140	9.2390892	3.6757077
H	5.4484409	6.1719154	6.2963759

Model $\mathbf{d^+}$:

C	3.6113995	4.7110964	3.8293861
C	3.7842065	5.1025737	5.2159902
C	5.0596021	5.7653990	5.3677980
C	5.6987906	5.7429804	4.0866162
C	4.8173955	5.1005454	3.1530164
Fe	3.9153604	6.7492207	3.9800104
C	3.3926905	7.9900894	2.4227898
C	4.3496215	8.6492844	3.2716778
C	3.7675678	8.7175519	4.5859217
C	2.4705005	8.1104447	4.5458243
C	2.2377219	7.6566065	3.2062064
C	5.6641855	9.2329761	2.8481774
N	2.8859920	4.8740490	6.2129937
C	2.2312152	4.4857325	7.1338506
Fe	0.8135589	4.6087777	8.4355950
C	-0.3921915	4.9760627	7.1884133
O	-1.1841011	5.2119605	6.3791814
C	2.4580038	3.9392166	3.2708251
Ni	2.6636474	2.6048736	8.1856835
S	3.1564314	1.2174107	6.4716782
C	4.8180167	1.4873924	6.9022134
N	5.8644374	0.8864511	6.3180038

C	7.2449713	1.1621512	6.7513018
C	7.9326633	2.2330983	5.9019544
S	4.9228297	2.6087066	8.2244325
S	2.4003551	3.8243398	10.0408277
C	1.4167147	2.7673358	11.2954365
N	0.9152848	1.5171546	10.8218278
C	-0.0860250	1.5692198	9.8054783
S	0.4526542	2.2703595	8.1081752
C	5.6704639	-0.0866460	5.2290339
C	5.5659767	-1.5288000	5.7301376
C	-0.5714738	4.6912376	9.7706323
N	-1.4118577	4.7378157	10.5891906
C	1.2258675	6.2926380	8.8055292
O	1.4864796	7.3924187	9.0506137
H	5.0122059	4.9497106	2.0937471
H	6.6745119	6.1635395	3.8578358
H	1.3499889	7.1394520	2.8513089
H	3.5338852	7.7683902	1.3674816
H	-0.9236640	2.1990034	10.1285131
H	-0.4306955	0.5569757	9.5643661
H	1.6676483	0.8666468	10.5861176
H	2.1348366	2.6014000	12.1067932
H	0.5912797	3.4065749	11.6309437
H	7.2062176	1.4712270	7.8052911
H	7.7961088	0.2109082	6.7079022
H	8.9592074	2.3912502	6.2627230
H	7.9896174	1.9374983	4.8445295
H	7.3916501	3.1860773	5.9669645
H	4.7584038	0.1982203	4.6857628
H	6.5161308	0.0301705	4.5353518
H	5.4397006	-2.2115142	4.8776794
H	6.4700770	-1.8346158	6.2758854
H	4.6997574	-1.6449756	6.3944236
H	1.5144650	4.2128337	3.7616642
H	2.3499526	4.1192281	2.1927123
H	2.6041133	2.8574413	3.4242093
H	4.2434640	9.1437584	5.4658642
H	1.7969789	7.9879964	5.3893519
H	6.1037904	8.6719919	2.0119725
H	5.5349059	10.2762570	2.5154141
H	6.3874140	9.2390892	3.6757077
H	5.4484409	6.1719154	6.2963759

Model $\mathbf{d^{+}\text{-}H_2}$:

C	3.5092861	4.7405899	3.7283913
C	3.7750451	5.0761034	5.1032100
C	5.0719159	5.6728170	5.1849596
C	5.6185939	5.7313361	3.8669856
C	4.6592531	5.1596552	2.9696471
Fe	3.8196229	6.7903397	3.9251872
C	3.5525798	8.7509975	4.6266116
C	2.2961215	8.0469556	4.5330111
C	2.1305235	7.6761532	3.1613083
C	3.2881152	8.1118082	2.4334686
C	4.1950568	8.7706238	3.3300328
C	5.4841405	9.4473529	2.9902808
N	4.0696563	9.2879727	5.7654378
C	4.4835810	9.8108029	6.7473704
Ni	3.7670517	12.1387664	7.3011478
S	1.5996657	11.8506243	6.6707219
C	2.0634361	12.5970679	5.1669284
N	1.2221182	12.9457744	4.1971775
C	1.6991431	13.6369973	2.9791860
C	1.6256097	15.1597466	3.0957441
C	2.3143696	4.0053772	3.2047822
Fe	5.4310243	10.0988836	8.3690167
S	3.5583339	11.1887461	9.3328592
C	4.2584550	12.4339079	10.5544556
N	4.9056069	13.5524039	9.9085436
C	6.1685788	13.3038907	9.2533787

S	5.9880202	12.2979392	7.6754327
C	6.4331379	10.2953598	9.9940867
N	7.0428690	10.4270455	10.9875899
C	4.8559088	8.5333676	9.0158987
O	4.4847597	7.5295582	9.4398641
C	6.9394506	9.4710551	7.6413841
O	7.9174975	9.0718248	7.1837330
S	3.7840792	12.8766606	5.1445052
C	-0.2318896	12.7047640	4.3165865
C	-0.6752034	11.4002683	3.6540725
H	3.4663287	7.9617489	1.3716026
H	1.2794735	7.1409830	2.7489565
H	6.5828889	6.1500873	3.5919616
H	4.7740591	5.0608118	1.8929180
H	6.8915336	12.7403311	9.8648901
H	6.6000446	14.2597324	8.9324701
H	4.9203405	14.3901019	10.4906853
H	3.3896462	12.7982518	11.1160312
H	4.9207168	11.8446365	11.2088537
H	-0.4835619	12.7060764	5.3864490
H	-0.7356311	13.5693281	3.8617728
H	-1.7634816	11.2884329	3.7565672
H	-0.4366542	11.3875083	2.5814575
H	-0.1954655	10.5349843	4.1303380
H	2.7312856	13.3100061	2.7911492
H	1.0831097	13.2724543	2.1448013
H	1.9705407	15.6165398	2.1579002
H	0.5983620	15.5046298	3.2776334
H	2.2669358	15.5227589	3.9092465
H	6.2130894	9.3725772	3.8081707
H	5.9316108	9.0114689	2.0883958
H	5.3144061	10.5190101	2.7984153
H	3.1002745	4.9016095	5.9374901
H	5.5435916	6.0504434	6.0881558
H	2.1071706	4.2605599	2.1570780
H	2.4947839	2.9193684	3.2492382
H	1.4158292	4.2132657	3.8007002
H	1.6082006	7.8744051	5.3550863
H	3.6663224	13.9413242	8.3482283
H	3.2084668	13.9889897	7.7109187

Model **d^+-2H:**

C	3.4860523	4.7359911	3.6095857
C	3.7372452	5.0065651	5.0001743
C	5.0313842	5.6068459	5.1218985
C	5.5922831	5.7234277	3.8094564
C	4.6412596	5.1876018	2.8802301
Fe	3.8132410	6.7670875	3.9136088
C	3.6057845	8.6407698	4.7070519
C	2.3185938	7.9892457	4.5945816
C	2.1236488	7.7055204	3.2062092
C	3.2802262	8.1491579	2.4825120
C	4.2278612	8.7217211	3.3961055
C	5.5245439	9.3912659	3.0672818
N	4.1443071	9.1342099	5.8629221
C	4.5910588	9.6167926	6.8432734
Ni	3.7162251	12.2848884	7.3395477
S	1.5635353	12.0331081	6.7457354
C	2.0236541	12.6992003	5.2046557
N	1.1892340	13.0008950	4.2152583
C	1.6787869	13.6110281	2.9598657
C	1.5927059	15.1374620	2.9708116
C	2.2912100	4.0345796	3.0397611
Fe	5.5118345	10.0337211	8.4579146
S	3.5893572	11.1370222	9.3113805
C	4.2202512	12.3962143	10.5112947
N	4.8770323	13.5496307	9.8175730
C	6.1813298	13.2878051	9.1316705
S	5.9685697	12.2164643	7.6375013

C	6.4713690	10.4157271	10.0708999
N	7.0329847	10.7207061	11.0553945
C	5.0012994	8.4828519	9.1890360
O	4.6691699	7.4912859	9.6683062
C	7.0411829	9.3953971	7.7879782
O	8.0326572	8.9921968	7.3659932
S	3.7459930	12.9527507	5.1848538
C	-0.2632607	12.7503396	4.3328329
C	-0.6851988	11.4136160	3.7220736
H	3.4365269	8.0456492	1.4116340
H	1.2565017	7.2089951	2.7791175
H	6.5607166	6.1489952	3.5610515
H	4.7620766	5.1394441	1.8007261
H	6.8832203	12.8106332	9.8264877
H	6.5570636	14.2557179	8.7785763
H	4.9757834	14.3406257	10.4688083
H	3.3462793	12.7974665	11.0386939
H	4.9267809	11.9231181	11.2039265
H	-0.5228534	12.7939536	5.4000514
H	-0.7721230	13.5900688	3.8389398
H	-1.7715900	11.2894422	3.8296047
H	-0.4468656	11.3625802	2.6506518
H	-0.1909755	10.5752020	4.2301491
H	2.7157864	13.2791995	2.8096723
H	1.0784787	13.1849006	2.1434859
H	1.9499311	15.5305823	2.0090863
H	0.5602193	15.4860452	3.1112909
H	2.2174196	15.5610735	3.7678493
H	6.2675228	9.2570030	3.8651816
H	5.9476867	8.9877152	2.1385895
H	5.3800775	10.4751019	2.9270246
H	3.0528593	4.7933231	5.8174644
H	5.4961615	5.9375617	6.0469172
H	2.0926397	4.3477014	2.0058919
H	2.4618028	2.9459530	3.0271828
H	1.3891576	4.2189627	3.6386216
H	1.6359369	7.7894174	5.4149988
H	3.4616291	13.7621845	7.9183518
H	4.1630936	13.8061184	8.9639943

Model $\mathbf{d_{TS}^{+}\text{-}H_2}$:

C	4.1852892	8.7343431	3.3932462
C	3.5790677	8.6482386	4.7101019
C	2.3037750	7.9724666	4.6145364
C	2.0976488	7.6805605	3.2294906
C	3.2382903	8.1417328	2.4916221
Fe	3.8092641	6.7681203	3.9164587
C	4.6487783	5.2006243	2.8726562
C	3.5073536	4.7321407	3.6132741
C	3.7703457	5.0031154	5.0017139
C	5.0580103	5.6184846	5.1107494
C	5.6028722	5.7458912	3.7931503
C	2.3161975	4.0153665	3.0551220
N	4.1244239	9.1454740	5.8601242
C	4.5677413	9.6261201	6.8439577
Fe	5.4851624	10.0158115	8.4665000
C	7.0128559	9.3644095	7.8045786
O	8.0038302	8.9535977	7.3886095
C	5.4673875	9.4236222	3.0488899
Ni	3.7304157	12.2461381	7.3456503
S	3.7603619	12.9508560	5.2018970
C	2.0399452	12.6784327	5.2106441
N	1.2071387	12.9879982	4.2224973
C	-0.2437003	12.7224408	4.3300144
C	-0.6499246	11.3877799	3.7044335
S	1.5772010	11.9809197	6.7369441
S	3.5741530	11.1336247	9.3233938
C	4.2116905	12.4100860	10.5111447
N	4.8645851	13.5427624	9.8053198
C	6.1731998	13.2692792	9.1576632
S	5.9846168	12.1918755	7.6570684

C	1.6943877	13.6297879	2.9818630
C	1.5961329	15.1548425	3.0277385
C	6.4369371	10.3717088	10.0907197
N	6.9955170	10.6542177	11.0833977
C	4.9456168	8.4661576	9.1789739
O	4.5938140	7.4738483	9.6427363
H	3.3842483	8.0390179	1.4192356
H	1.2335572	7.1690646	2.8140613
H	6.5629674	6.1846885	3.5356987
H	4.7590406	5.1560104	1.7918872
H	6.8628592	12.7791381	9.8571070
H	6.5745765	14.2272123	8.8058636
H	4.9339246	14.3599385	10.4246225
H	3.3360522	12.8099116	11.0366564
H	4.9091075	11.9261970	11.2070490
H	-0.5096350	12.7534945	5.3960910
H	-0.7575535	13.5620093	3.8410821
H	-1.7358542	11.2531135	3.8037804
H	-0.4040939	11.3486421	2.6342155
H	-0.1518252	10.5491223	4.2083569
H	2.7341132	13.3096447	2.8257571
H	1.0984401	13.2175918	2.1552060
H	1.9505651	15.5731469	2.0756432
H	0.5608165	15.4915134	3.1759647
H	2.2171821	15.5648221	3.8346938
H	6.2192793	9.3068241	3.8411362
H	5.8888281	9.0227772	2.1183378
H	5.3026564	10.5040345	2.9053183
H	3.0977408	4.7798315	5.8260544
H	5.5280345	5.9541061	6.0313018
H	2.1033024	4.3256823	2.0233263
H	2.5015955	2.9292106	3.0407090
H	1.4177976	4.1871099	3.6630933
H	1.6344185	7.7638294	5.4436571
H	3.4852767	13.7496690	7.9405247
H	4.1012320	13.7597635	8.8366250

Model **e**:

C	5.5434218	5.6825439	4.1765084
C	4.5525935	5.1503320	3.2778994
C	3.3372054	4.9371160	4.0309169
C	3.6197858	5.3211790	5.4035168
C	4.9761333	5.8080069	5.4833444
Fe	3.9033908	6.9126963	4.1257953
C	2.4041529	8.3003394	4.4377719
C	2.5318585	8.0089765	3.0404684
C	3.8669346	8.3468021	2.6408032
C	4.5767164	8.8474353	3.7869829
C	3.6613737	8.8122178	4.8971158
H	1.7583829	7.5901033	2.4019819
C	5.9776736	9.3802242	3.8074937
C	2.0279322	4.3780037	3.5517275
N	1.8155252	2.9780591	3.9472128
C	0.4465693	2.5602581	3.6607947
N	2.7436710	5.2569436	6.4409968
C	2.0822023	5.1124140	7.4245176
Ni	2.4331514	3.5750113	8.9306427
S	4.6894586	3.5690772	9.1185659
C	4.6200783	2.0922035	8.2042824
N	5.6693840	1.2916264	7.9605287
C	7.0191997	1.6269233	8.4426921
C	7.8767285	2.3191893	7.3809428
C	2.7820601	2.0724674	3.3388422
Fe	0.6171643	5.5955947	8.6005991

C	-0.8304178	6.0140201	9.7974961
N	-1.7106655	6.2599901	10.5345575
S	0.2187260	3.2563295	8.8225431
C	-0.4517865	2.9703814	10.5289167
C	0.5557083	3.1388204	11.6611854
C	1.0841258	4.5583405	11.8368512
S	2.1017914	5.2034578	10.4256234
S	2.9944940	1.7670276	7.6987932
C	1.0809811	7.3055021	8.5826943
O	1.3807558	8.4229964	8.5748571
C	-0.5046396	5.7005226	7.2347513
O	-1.2364577	5.7823227	6.3416064
C	5.4972881	0.0219232	7.2339792
C	5.2037946	-1.1600289	8.1616730
C	4.7793258	4.8322865	1.8300303
H	6.5551123	5.9675849	3.8961788
H	4.2839829	8.2273541	1.6433734
H	-1.3045196	3.6524198	10.6510497
H	-0.8196992	1.9351834	10.4990018
H	1.3972107	2.4406311	11.5211614
H	0.0512021	2.8526120	12.6017185
H	1.7655983	4.6070849	12.6977351
H	0.2631849	5.2730715	11.9861686
H	6.9047690	2.2707373	9.3258091
H	7.4889325	0.6898201	8.7778755
H	8.8755214	2.5318924	7.7884556
H	8.0036231	1.6894419	6.4890150
H	7.4203441	3.2693103	7.0731197
H	4.6776600	0.1580786	6.5143270
H	6.4173702	-0.1494391	6.6560574
H	5.0939194	-2.0807487	7.5707656
H	6.0159588	-1.3184501	8.8854572
H	4.2698025	-0.9920750	8.7135633
H	1.9577733	4.5069227	2.4458138
H	3.8921537	9.1108099	5.9166123
H	1.5195571	8.1379113	5.0474320
H	6.5997340	8.9085032	3.0343262
H	5.9806440	10.4665960	3.6185727
H	6.4572488	9.2143315	4.7822061
H	5.4562398	6.1777024	6.3842505
H	1.2055788	4.9631736	3.9901635
H	2.6142140	1.0534053	3.7156156
H	2.7109151	2.0450309	2.2260269
H	3.8017204	2.3730359	3.6137944
H	0.2894960	1.5380347	4.0328782
H	-0.2625778	3.2223426	4.1762919
H	0.2065323	2.5714268	2.5724408
H	5.1113658	3.7884618	1.7016976
H	3.8653388	4.9607427	1.2349985
H	5.5564402	5.4818610	1.4039736

Model $\mathbf{e}^{+}$:

C	5.5256858	5.8404744	3.9962821
C	4.5194218	5.2616821	3.1495083
C	3.3478831	5.0191604	3.9503403
C	3.6698710	5.4328868	5.3017423
C	5.0121770	5.9655887	5.3250689
Fe	3.8549075	7.0599368	4.0285580
C	2.3217584	8.4077193	4.3541309
C	2.4485148	8.1460520	2.9512035
C	3.7623691	8.5452836	2.5488259
C	4.4591687	9.0635733	3.6898285
C	3.5633557	8.9633442	4.8091800
H	1.6867363	7.7126653	2.3087008
C	5.8376877	9.6464361	3.7045697
C	2.0383351	4.4119108	3.5306193
N	1.8971816	3.0131692	3.9593631
C	0.5249479	2.5451811	3.7586430
N	2.8437868	5.3315289	6.3782615
C	2.1654458	5.1874538	7.3443108
Ni	2.4713990	3.5381076	8.8675460
S	4.7260555	3.5058770	9.0795291
C	4.6287899	1.9726916	8.2580259

N	5.6374765	1.1184262	8.1127970
C	6.9892595	1.4265842	8.6279411
C	7.9096047	2.0182296	7.5595282
C	2.8597505	2.1266127	3.3089767
Fe	0.7505818	5.5729296	8.5872953
C	-0.6913381	6.0096970	9.7740500
N	-1.5714537	6.2643013	10.5061860
S	0.2522121	3.2726426	8.7212756
C	-0.4224135	2.9289281	10.4148728
C	0.5809762	3.0368088	11.5575976
C	1.1405795	4.4352007	11.7934987
S	2.1749036	5.1261199	10.4168783
S	2.9932069	1.6818462	7.7212011
C	1.2317742	7.2959396	8.6527371
O	1.5355299	8.4058371	8.6994722
C	-0.4187385	5.7440832	7.2455762
O	-1.1811929	5.8562177	6.3891936
C	5.4409241	-0.2020733	7.4745131
C	5.1353604	-1.3073038	8.4872561
C	4.6920133	4.9474172	1.6946959
H	6.5160407	6.1491764	3.6701413
H	4.1775292	8.4523803	1.5480249
H	-1.2658789	3.6198607	10.5524580
H	-0.8078449	1.9031446	10.3378441
H	1.4032767	2.3186882	11.4092960
H	0.0589257	2.7333062	12.4816006
H	1.8243942	4.4348678	12.6533828
H	0.3398985	5.1662999	11.9714855
H	6.8731897	2.1197034	9.4724834
H	7.3996333	0.4882951	9.0266680
H	8.8999465	2.2089392	7.9954938
H	8.0438564	1.3321235	6.7119447
H	7.5123724	2.9696821	7.1823889
H	4.6233547	-0.1032878	6.7472958
H	6.3585395	-0.4225536	6.9111122
H	5.0226538	-2.2649256	7.9606213
H	5.9444659	-1.4236466	9.2215912
H	4.2009689	-1.0986598	9.0242170
H	1.9223122	4.5199184	2.4280540
H	3.7934582	9.2650165	5.8278885
H	1.4429723	8.2178156	4.9639124
H	6.4724142	9.2113194	2.9214908
H	5.7836764	10.7312835	3.5192080
H	6.3296563	9.5042264	4.6757826
H	5.5259075	6.3470722	6.2023241
H	1.2139172	4.9764558	3.9911160
H	2.7313498	1.1069023	3.6957884
H	2.7360899	2.0931584	2.2038286
H	3.8848397	2.4481620	3.5364475
H	0.4286044	1.5233132	4.1493794
H	-0.1754216	3.1886795	4.3080951
H	0.2233578	2.5342719	2.6888434
H	5.0570651	3.9157196	1.5668479
H	3.7496068	5.0321980	1.1389277
H	5.4284963	5.6163636	1.2306656

Model **e^+-2H**:

C	4.0109529	9.4556436	4.2690573
C	3.1186031	9.7147932	5.3657559
C	1.7862047	9.8674924	4.8135926
C	1.8993295	9.6939022	3.3709311
C	3.2749776	9.4297742	3.0433409
Fe	2.5317799	8.0223457	4.3408201
C	1.4509788	6.4101742	3.6167958
C	1.2312709	6.5654057	5.0231107
C	2.4993907	6.4503339	5.6829030
C	3.5136100	6.2186090	4.6907405
C	2.8524751	6.2029703	3.4127794
C	4.9650807	5.9478534	4.9440874
C	0.5125899	10.1570899	5.5253356
N	0.0936383	11.6326670	5.4985648
C	1.1222771	12.5456372	6.0769983
N	0.8574095	9.8250619	2.4955372

C	-0.1273512	10.1163287	1.9036262
Fe	-1.6433429	10.3145759	0.8434548
C	-3.1692695	10.4008045	-0.3272468
N	-4.0957306	10.4126752	-1.0463729
C	-0.8292389	9.4875101	-0.5198511
O	-0.3083340	8.9663588	-1.4040010
C	-2.4091359	8.8575861	1.5439279
O	-2.9107494	7.9314918	2.0129122
S	-0.8562182	12.4551645	0.1979055
Ni	-1.0161752	13.2851690	2.3328639
S	-1.7125692	14.7917702	3.9640759
C	-0.4258279	15.7995402	3.3445162
N	-0.1810160	17.0458996	3.7511539
C	0.9181569	17.8429435	3.1644850
C	2.2177004	17.7397611	3.9645415
S	-2.6852405	11.7819765	2.4068120
C	-3.9596345	12.7378473	1.4341549
C	-3.3718927	13.7948198	0.4955879
C	-2.3340464	13.3287029	-0.5288727
S	0.4635449	14.9757365	2.0956251
C	-1.0219317	17.7076695	4.7718686
C	-2.1554982	18.5327040	4.1606470
C	-1.2388751	11.8116492	6.1526176
C	3.5278526	9.8653118	6.8008845
H	5.0789494	9.2757469	4.3635055
H	0.2712843	6.7334423	5.5049334
H	2.6716829	6.5229039	6.7540592
H	-4.5620032	11.9957825	0.8972866
H	-4.5763492	13.2270286	2.2005252
H	-2.9384982	14.6088744	1.1019945
H	-4.2126853	14.2401220	-0.0637285
H	-1.9076922	14.2013323	-1.0421074
H	-2.7656370	12.6469191	-1.2708132
H	1.0671826	17.4991557	2.1315215
H	0.5666162	18.8832591	3.1165726
H	2.9856148	18.3743154	3.5009596
H	2.0843766	18.0789663	5.0013727
H	2.5907484	16.7069754	3.9754572
H	-1.4245522	16.9263516	5.4309445
H	-0.3531703	18.3391768	5.3739222
H	-2.7278159	19.0203553	4.9619019
H	-1.7746775	19.3200827	3.4954287
H	-2.8409369	17.8926634	3.5901139
H	-0.0289139	12.3819865	3.1500582
H	-0.3276401	9.6170090	5.0686467
H	0.5709975	9.8735106	6.5851403
H	3.3428557	6.0668092	2.4520867
H	0.6932124	6.4628489	2.8396224
H	5.3207878	6.4506979	5.8533971
H	5.1273581	4.8666250	5.0817375
H	5.5917942	6.2681882	4.1009650
H	3.6641548	9.2549234	2.0449521
H	0.7736498	13.5765449	5.9503065
H	1.2549855	12.3171320	7.1417063
H	2.0635471	12.4040267	5.5363383
H	-1.5257085	12.8661042	6.0726429
H	-1.9779464	11.1946409	5.6287580
H	-1.1689049	11.5112815	7.2053777
H	-0.0200554	11.9377233	4.4523775
H	3.7964434	10.9092859	7.0328021
H	2.7330054	9.5607639	7.4965372
H	4.4101997	9.2499908	7.019683

Model $^{disp}\mathbf{b}^{-}$:

C	6.4702769	4.2733249	4.1809208
N	6.3939829	4.3591290	5.3514349
Fe	6.4417490	4.3429097	2.2251744

C	6.4066876	6.1060864	2.3185864
O	6.3836839	7.2652781	2.3724340
S	8.8326766	4.2808289	2.2871443
Ni	8.4854887	2.4935247	3.5630201
S	9.8290297	3.1320846	5.2420246
C	8.6535543	2.1231009	6.0359192
N	8.1264703	2.4082695	7.2343310
C	7.0913748	1.5576965	7.8416065
C	5.6834861	2.0016539	7.4444770
C	9.3551815	3.5947599	0.6426981
C	9.1257825	2.0928454	0.4841935
C	7.6653102	1.6509104	0.5404001
S	6.8362520	1.9824018	2.1683302
C	6.4115885	4.4563259	0.3027999
N	6.3897924	4.5314775	-0.8705259
C	4.6910386	4.1117557	2.2478155
O	3.5406814	3.9555982	2.2592247
S	8.0762131	0.8211970	5.0195752
C	8.3776125	3.7002944	7.8919693
C	9.6481961	3.6710510	8.7415782
H	8.8181559	4.1572653	-0.1333889
H	10.4328212	3.8089872	0.5750782
H	9.6896434	1.5600231	1.2697295
H	9.5359745	1.7885102	-0.4978766
H	7.6066487	0.5594302	0.4084748
H	7.0733655	2.1489383	-0.2396832
H	7.2736165	0.5205221	7.5268465
H	7.2373481	1.6147997	8.9332313
H	4.9364968	1.3595997	7.9391290
H	5.5090815	3.0497055	7.7248178
H	5.5714565	1.9338018	6.3548152
H	8.4272728	4.4673029	7.1064848
H	7.4915760	3.9181577	8.5048094
H	9.7882254	4.6388974	9.2488860
H	9.5931760	2.8798216	9.5070487
H	10.5225179	3.4823708	8.1018234
H	5.6505169	5.3624847	7.4413433
H	5.4257929	5.6443928	8.1076309

Model $^{solv}\mathbf{b}^{-}$:

C	7.8251196	1.7559834	0.7272223
C	9.2221594	2.3140401	0.9792228
C	9.3405995	3.8345997	0.9374670
S	8.3381220	4.7326531	2.2227561
Fe	6.0524826	4.5625693	1.5590666
C	5.5646349	4.7249357	3.4494786
N	5.0849611	4.9669253	4.4978868
Ni	7.6334513	3.2026877	3.6703401
S	7.0188332	1.7276772	5.2638515
C	7.9189809	2.7332893	6.3624518
N	7.9849990	2.5581035	7.6850783
C	8.7785283	3.4609044	8.5404629
C	10.1895568	2.9336708	8.8074841
S	6.5446340	2.2642469	1.9778363
S	8.7012806	4.0150984	5.4821334
C	6.5015675	4.4296490	-0.3069336
N	6.7209238	4.3916560	-1.4628717
C	4.3703168	4.1853719	1.1822836
O	3.2663483	3.9289148	0.9305010
C	5.9076218	6.3145025	1.4031117
O	5.8162631	7.4675210	1.3023749
C	7.2524838	1.4630132	8.3499901
C	5.8660108	1.8917827	8.8333598
H	9.0401797	4.2346464	-0.0397818
H	10.3783248	4.1344592	1.1391887
H	9.5894738	1.9470813	1.9514181
H	9.8933365	1.9037573	0.2029371
H	7.8448555	0.6586996	0.7830970
H	7.4457382	2.0528600	-0.2590586
H	7.1744774	0.6302185	7.6378755

H	7.8743815	1.1217286	9.1899232
H	5.3750376	1.0475920	9.3383871
H	5.9291199	2.7254703	9.5470717
H	5.2383846	2.2015972	7.9867727
H	8.8167835	4.4408514	8.0455546
H	8.2223592	3.5870366	9.4805249
H	10.7265521	3.6355698	9.4615071
H	10.1663649	1.9546973	9.3071663
H	10.7531231	2.8365450	7.8695672

Model $^{\mathbf{disp}}\mathbf{b}$:

C	4.6786573	5.4048625	2.2649623
N	3.9297719	5.7653967	3.0990168
Fe	5.9093783	4.7580905	0.9471230
C	6.0116388	6.3951178	0.2355630
O	6.0947416	7.4538914	-0.2112919
S	7.6969231	5.1775836	2.4285583
Ni	6.9252975	3.7493674	3.9976329
S	8.4172568	4.2594913	5.6740060
C	7.8048812	2.8246202	6.4531506
N	8.1915599	2.3958934	7.6544349
C	7.5818661	1.2089099	8.2836792
C	6.3469557	1.5937213	9.0989730
C	9.0798319	4.0901400	1.8229808
C	8.8935087	2.5906589	2.0871483
C	7.5927414	1.9368616	1.6034354
S	6.0187589	2.7570832	2.1758706
C	7.0718745	4.1194058	-0.4453259
N	7.7909822	3.7154111	-1.2815309
C	4.5246317	4.1920839	-0.0342891
O	3.6363981	3.8074534	-0.6588608
S	6.6023795	2.0307343	5.4742613
C	9.2169532	3.0979804	8.4465212
C	10.5962688	2.4703018	8.2482041
H	9.1846194	4.2995883	0.7511975
H	9.9718763	4.4377222	2.3637550
H	9.0074097	2.4041062	3.1693197
H	9.7255520	2.0663879	1.5852627
H	7.5401433	0.9140047	2.0026225
H	7.5389918	1.9177682	0.5076637
H	7.3249930	0.4895736	7.4935983
H	8.3576417	0.7531523	8.9166612
H	5.9244763	0.7033640	9.5871692
H	6.6051998	2.3276131	9.8767091
H	5.5825268	2.0286411	8.4398112
H	9.2178816	4.1563012	8.1508383
H	8.8981345	3.0404439	9.4985420
H	11.3372838	2.9830166	8.8789399
H	10.5862659	1.4051082	8.5245366
H	10.9060056	2.5603207	7.1974938
H	5.3736244	4.7972287	4.2128024
H	5.8040001	4.7281511	4.8832376

Model $^{\mathbf{solv}}\mathbf{b}$:

C	4.6552405	5.3845219	2.2563713
N	3.8634118	5.7721666	3.0363369
Fe	5.8900105	4.7550518	0.9239373

C	5.9485068	6.3957352	0.2326623
O	5.9975514	7.4623806	-0.2063000
S	7.7069582	5.1693169	2.3903527
Ni	6.9792189	3.7126654	3.9875926
S	8.4250439	4.2461176	5.6875207
C	7.8152934	2.8078373	6.4751140
N	8.1775950	2.3930308	7.6795323
C	7.5318486	1.2211668	8.3156100
C	6.3341895	1.6269460	9.1754863
C	9.1024085	4.1042450	1.7720571
C	8.9329774	2.6080270	2.0495281
C	7.6475157	1.9364216	1.5579487
S	6.0648760	2.7373165	2.1370702
C	7.0290616	4.1585360	-0.5094906
N	7.6776898	3.8262191	-1.4317032
C	4.4972067	4.1944879	-0.0351612
O	3.5966427	3.8195152	-0.6523539
S	6.6471161	1.9993768	5.4581506
C	9.2256019	3.0876972	8.4603026
C	10.5935564	2.4216368	8.3110754
H	9.1996328	4.3184596	0.7018329
H	9.9923444	4.4754183	2.2976499
H	9.0433134	2.4283990	3.1329350
H	9.7800276	2.0857127	1.5729614
H	7.5998206	0.9109365	1.9472477
H	7.5882839	1.9112972	0.4638345
H	7.2310475	0.5259435	7.5207844
H	8.3028205	0.7215523	8.9168234
H	5.9034126	0.7290867	9.6394351
H	6.6297296	2.3168338	9.9775913
H	5.5567927	2.1070148	8.5659688
H	9.2574205	4.1330722	8.1256611
H	8.8947775	3.0842804	9.5078797
H	11.3247624	2.9613172	8.9284917
H	10.5724870	1.3761140	8.6479243
H	10.9350097	2.4487261	7.2675005
H	5.4503869	4.6969117	4.2301200
H	5.8982922	4.7360601	4.888101

Model ^{disp}**c**:

C	3.9128065	4.2936312	3.5428342
C	4.4138648	4.4337182	4.8792266
C	5.6767223	5.1203207	4.8200311
C	5.9774205	5.4313761	3.4493611
C	4.8911519	4.8837123	2.6634726
Fe	4.1943730	6.2521146	4.0033411
C	2.4015810	7.1827824	3.6942661
C	3.4316928	7.7987842	2.9069837
C	4.4512621	8.2648973	3.8030710
C	4.0434536	7.9388467	5.1416916
C	2.7748591	7.2624276	5.0820697
C	1.9780434	6.7583064	6.2455311
C	7.1833384	6.1188709	2.8996975
N	4.8079692	4.9591540	1.3036082
C	5.0350649	4.6068716	0.1790977
Fe	5.1093522	4.8207696	-1.7177148
C	5.2729421	4.9591280	-3.6290352
N	5.3957732	5.0093417	-4.7948825
C	3.4013941	5.2927396	-1.8109731
O	2.2894215	5.6036299	-1.8642525
C	5.7449509	6.4661159	-1.5452595
O	6.1624247	7.5371860	-1.4204194
S	7.3250575	3.9276670	-1.5317599
Ni	5.9899773	2.7048685	-0.2190338
S	7.3544560	2.7235685	1.5807935
C	6.1128031	1.7959111	2.3652757
N	6.1430476	1.4141567	3.6451999
C	5.1903138	0.4322556	4.1857238
C	4.0052333	1.0881003	4.8914601

S	4.5116676	2.5102736	-1.8780998
C	5.3751200	1.8484153	-3.3748114
C	6.8821317	1.6788305	-3.2149189
C	7.6451500	2.9934290	-3.0959931
S	4.8365273	1.4243183	1.2465981
C	7.1711767	1.9173493	4.5688492
C	8.4128813	1.0251028	4.5861151
H	6.2880049	5.4095059	5.6716659
H	3.9037927	4.1101167	5.7824517
H	5.3855959	8.7387283	3.5142390
H	4.6129671	8.1272498	6.0485434
H	7.4003297	3.6648086	-3.9310066
H	8.7280402	2.8020330	-3.0804590
H	7.0962206	1.0420445	-2.3399427
H	7.2563793	1.1545792	-4.1125994
H	4.9015765	0.8715458	-3.5510638
H	5.1448798	2.5261987	-4.2089947
H	4.8463566	-0.2007751	3.3554349
H	5.7596327	-0.2053518	4.8805782
H	3.3502625	0.3137753	5.3185939
H	4.3484468	1.7470147	5.7020712
H	3.4314387	1.6921800	4.1769347
H	7.4174208	2.9457850	4.2684382
H	6.7001862	1.9690367	5.5622565
H	9.1481596	1.4129096	5.3071850
H	8.1520854	-0.0037187	4.8783182
H	8.8750738	1.0035745	3.5892137
H	6.9300007	6.6658786	1.9798660
H	7.5922988	6.8310816	3.6309475
H	7.9635865	5.3824489	2.6448098
H	1.5076246	6.6982386	3.3092625
H	3.4624718	7.8487223	1.8217597
H	2.6368305	6.4868031	7.0834866
H	1.2744076	7.5295833	6.6036087
H	1.3902516	5.8722300	5.9633874
H	2.9853573	3.8301550	3.2227862

Model $^{disp}\mathbf{c}^{+}$:

C	3.6418993	4.5048768	3.6069999
C	4.0158282	4.6583825	4.9827232
C	5.3385589	5.2172706	5.0298902
C	5.8154328	5.4194090	3.6929777
C	4.7706875	4.9427511	2.8196109
Fe	4.0377510	6.4616340	4.0317257
C	2.4713795	7.5918024	3.3527097
C	3.7149518	8.1614118	2.9126159
C	4.4819542	8.4904375	4.0743326
C	3.7131876	8.1302985	5.2262889
C	2.4617995	7.5768407	4.7927727
C	1.3480405	7.0977305	5.6683671
C	7.1306201	5.9695255	3.2521884
N	4.8195906	4.9843433	1.4606898
C	5.0545849	4.6486589	0.3381242
Fe	5.1115995	4.7516947	-1.5551974
C	5.1426098	4.9245631	-3.4657891
N	5.1839676	4.9843129	-4.6355675
C	3.3788802	5.2224990	-1.6019840
O	2.2686936	5.5186986	-1.6311052
C	5.7868379	6.4135785	-1.4683735
O	6.2231667	7.4757255	-1.4115323
S	7.3189014	3.9004719	-1.5599603
Ni	6.0082197	2.7482344	-0.1678813
S	7.5247359	2.6763239	1.4980272
C	6.3465902	1.7180638	2.3561803
N	6.5140374	1.2205155	3.5741962
C	5.4902807	0.3703595	4.2129788
C	4.5279592	1.2044397	5.0573220
S	4.4458129	2.4885050	-1.7364538
C	5.2325458	1.8097595	-3.2639410
C	6.7439902	1.6314508	-3.1839772
C	7.5257511	2.9390516	-3.1249888

S	4.9369259	1.4756994	1.3608314
C	7.7444612	1.4648839	4.3528857
C	8.7758690	0.3604005	4.1254393
H	5.8838009	5.4936399	5.9287892
H	3.3902624	4.4193358	5.8380077
H	5.4902194	8.8963858	4.0801106
H	4.0370285	8.2136896	6.2608198
H	7.2402677	3.6103083	-3.9478335
H	8.6061628	2.7412307	-3.1705634
H	7.0056436	0.9939688	-2.3237490
H	7.0606328	1.1003269	-4.0980798
H	4.7381826	0.8375657	-3.4033130
H	4.9545346	2.4837214	-4.0875551
H	4.9544034	-0.1782891	3.4254070
H	6.0318263	-0.3647471	4.8260402
H	3.7919058	0.5483168	5.5439057
H	5.0713158	1.7577018	5.8375655
H	3.9990869	1.9274060	4.4214867
H	8.1453727	2.4471963	4.0648367
H	7.4396052	1.5207135	5.4083186
H	9.6665951	0.5485840	4.7419872
H	8.3668921	-0.6221715	4.4030816
H	9.0786475	0.3337252	3.0694834
H	7.0189029	6.5661202	2.3354111
H	7.5743502	6.5991871	4.0350854
H	7.8266121	5.1449395	3.0228348
H	1.6722949	7.2234145	2.7145060
H	4.0341610	8.2840116	1.8807679
H	1.7286667	6.7389865	6.6351457
H	0.6458458	7.9235173	5.8701669
H	0.7824210	6.2887484	5.1848528
H	2.7113416	4.1132147	3.2082742

Model $^{disp}\mathbf{c}^{+}$-$\mathbf{H}_2$:

C	3.3804372	9.6035371	3.5580397
C	4.0107495	9.2366309	4.7891853
C	3.0054144	9.1782201	5.8141180
C	1.7305066	9.5106676	5.2423509
C	1.9831555	9.7910188	3.8468681
Fe	2.5664826	7.8606353	4.3104512
C	3.1578925	6.2628670	3.1123592
C	1.7570244	6.5113215	2.9688637
C	1.1495631	6.3851258	4.2629768
C	2.1881904	6.0569950	5.1997593
C	3.4374501	5.9780040	4.4900941
C	4.7722148	5.6490236	5.0791045
C	0.4080427	9.6141418	5.9282228
N	1.0131707	10.1302269	2.9486628
C	0.0766114	10.4113399	2.2818981
Fe	-1.4314375	10.5499364	1.2104217
C	-3.0074405	10.4858502	0.1117500
N	-3.9706351	10.4254360	-0.5533016
C	-0.6493393	9.5925310	-0.0935810
O	-0.1470926	8.9932406	-0.9373461
C	-2.1894034	9.1766802	2.0810299
O	-2.6873869	8.3087930	2.6506438
S	-2.3851708	12.1421644	2.6749168
Ni	-0.7750286	13.6680106	2.2304850
S	-1.2902293	15.1340994	3.8955286
C	-0.3809512	16.2996795	2.9663904
N	-0.2475941	17.5814354	3.2824702
C	0.5131806	18.5198236	2.4312744
C	1.9743624	18.6081353	2.8706885
S	-0.7335841	12.5911895	0.2464212
C	-2.2841932	13.3541509	-0.4520812
C	-3.2654236	13.9011672	0.5895503
C	-3.7449841	12.9507158	1.6908870
S	0.3029057	15.5513363	1.5461663
C	-0.8644227	18.1548156	4.4960823

C	-2.2503405	18.7257025	4.1966545
H	3.1668591	8.9034665	6.8530965
H	5.0648923	9.0063190	4.9148318
H	0.0980809	6.5301409	4.4956081
H	2.0655405	5.9135969	6.2704296
H	-4.3660796	12.1390455	1.2935892
H	-4.3144902	13.5234567	2.4364355
H	-2.8214063	14.7949244	1.0604010
H	-4.1616694	14.2416025	0.0426136
H	-1.9180832	14.1859532	-1.0703013
H	-2.7448371	12.5923245	-1.0917270
H	0.4314423	18.1852519	1.3875140
H	0.0086131	19.4935142	2.5136998
H	2.5062499	19.3410300	2.2470956
H	2.0508044	18.9286226	3.9202806
H	2.4651661	17.6310813	2.7597597
H	-0.9154403	17.3690636	5.2631773
H	-0.1771485	18.9348559	4.8557574
H	-2.6699138	19.1821694	5.1044547
H	-2.1967978	19.4993788	3.4159139
H	-2.9263645	17.9270602	3.8604115
H	0.8451264	12.9318959	2.7195744
H	0.4187242	12.8638385	3.3725436
H	-0.4148950	9.4088466	5.2290408
H	0.3457918	8.9030452	6.7629432
H	0.2619049	10.6282853	6.3361078
H	3.9021382	6.3298633	2.3226728
H	1.2510398	6.7919465	2.0488445
H	4.8433184	5.9949974	6.1200418
H	4.9257775	4.5570649	5.0776962
H	5.5865751	6.1024073	4.4965960
H	3.8453522	9.7129580	2.5828952

Model $^{disp}\mathbf{c}_{TS}^{+}$-$\mathbf{H}_2$:

C	1.6764955	6.6104085	3.1283635
C	1.8112716	6.3496279	4.5322362
C	3.2064999	6.1957675	4.8173176
C	3.9476478	6.3550221	3.6008607
C	2.9952319	6.6194907	2.5573083
Fe	2.8126382	8.0710029	4.0005019
C	4.1106837	9.5981020	4.4841059
C	3.0791436	9.5194424	5.4765521
C	1.8053653	9.6971829	4.8528871
C	2.0725703	9.8945190	3.4449902
C	3.4973567	9.8222899	3.2097705
H	3.2280685	9.3071041	6.5323104
C	0.4557689	9.7142157	5.4922076
N	1.1134132	10.1292452	2.5035616
C	0.2175974	10.4028857	1.7811720
Fe	-1.1319305	10.6001408	0.5271347
C	0.0074978	10.2424115	-0.8157891
O	0.7347214	10.0308261	-1.6814787
H	5.1752772	9.4714390	4.6602832
H	1.0022279	6.3102400	5.2567954
H	3.6441786	6.0361185	5.7997279
C	5.4318662	6.2644743	3.4444510
C	-1.6852619	8.9160243	0.8051211
O	-2.0488862	7.8407099	0.9983840
S	-2.6160927	11.4652159	2.1552401
C	-3.9463862	12.3412841	1.1854947
C	-3.5082917	13.6584888	0.5366360
C	-2.2939696	13.6299122	-0.3966137
S	-0.7388919	12.9281046	0.3549342
Ni	-1.3092414	13.2608008	2.5046461
S	-0.4354463	15.3363250	2.7263989
C	-1.4158539	15.4471527	4.1690424
N	-1.5600420	16.5452249	4.9002878

C	-2.4381800	16.5827276	6.0879185
C	-3.8441708	17.0577932	5.7211018
C	-2.4835942	10.6495741	-0.8395014
N	-3.3008419	10.6653500	-1.6794132
S	-2.2153994	13.9275918	4.4809409
C	-0.8823397	17.8120213	4.5549557
C	0.4539702	17.9460629	5.2837670
H	-4.3201544	11.6227102	0.4469794
H	-4.7271857	12.5504477	1.9298418
H	-3.3290875	14.4050579	1.3297408
H	-4.3641282	14.0254372	-0.0564062
H	-2.0214280	14.6609150	-0.6629934
H	-2.4882128	13.0520021	-1.3079901
H	-0.7459160	17.8461509	3.4650169
H	-1.5738572	18.6207228	4.8332123
H	0.9138086	18.9151985	5.0416739
H	0.3144994	17.8942036	6.3736993
H	1.1397545	17.1452514	4.9733957
H	-2.4625317	15.5785776	6.5337060
H	-1.9595673	17.2620043	6.8085999
H	-4.4657088	17.1159647	6.6261482
H	-3.8145547	18.0557312	5.2591810
H	-4.3119063	16.3539511	5.0183649
H	0.6369848	12.6811244	3.4416858
H	0.1906651	12.2620732	3.8920275
H	-0.3172728	9.3749366	4.7882062
H	0.4351390	9.0687738	6.3805038
H	0.1952742	10.7370982	5.8118748
H	3.2430453	6.8121173	1.5165016
H	0.7462755	6.7929744	2.5964699
H	5.9480157	6.5456067	4.3732606
H	5.7206476	5.2283655	3.2010840
H	5.7862101	6.9101050	2.6286601
H	3.9879433	9.9347705	2.2477904

Model ^{disp}**c'**:

O	7.1103612	-5.0667039	-1.4204885
C	4.9002720	-0.8820079	-0.2063596
Fe	5.5787115	-2.6258633	-0.6728783
C	6.7396150	-1.7349269	-1.7794814
N	7.4616562	-1.1137326	-2.4774528
C	6.2807472	-4.2802700	-1.1840061
Ni	4.1441821	-4.7842014	-1.3885654
S	4.2620418	-6.0750467	-3.2363162
C	4.3383221	-7.4141000	-2.1326584
N	4.4622464	-8.6986703	-2.4930824
C	4.5406441	-9.7674990	-1.4812283
C	5.9784217	-10.0905651	-1.0693122
N	4.5117673	0.1941156	0.0596577
S	4.2203783	-6.8550602	-0.4932603
S	3.8659152	-3.7281929	0.5566673
C	2.3591284	-2.6471765	0.5007896
C	1.6515097	-2.5856410	-0.8477334
C	2.4629422	-1.9231784	-1.9546222
S	3.9988487	-2.8308307	-2.4651645
C	4.5298774	-9.0895018	-3.9117526
C	3.1618008	-9.4505837	-4.4941214
C	6.6137144	-2.5671476	0.7606184
O	7.2810772	-2.5189526	1.7047924
H	2.7766201	-0.9111050	-1.6636608
H	1.8709428	-1.8648441	-2.8788299
H	1.3468121	-3.5980312	-1.1591370
H	0.7262371	-1.9965861	-0.7128981
H	1.6950864	-3.0824988	1.2607479
H	2.6746371	-1.6475311	0.8296307
H	3.9524687	-9.4463821	-0.6096781

H	4.0425758	-10.6517947	-1.9052591
H	5.9795301	-10.8993112	-0.3245324
H	6.5809839	-10.4209204	-1.9274626
H	6.4593782	-9.2106311	-0.6227220
H	4.9770093	-8.2520942	-4.4657645
H	5.2253954	-9.9390671	-3.9812473
H	3.2709555	-9.7515568	-5.5458515
H	2.6985905	-10.2863368	-3.9506345
H	2.4839016	-8.5879595	-4.4519902
C	8.1782737	-0.3093420	-3.3236132
C	7.6821151	0.8982487	-3.9408512
C	8.7110411	1.3705874	-4.8158881
C	9.8308911	0.4776372	-4.7231053
C	9.5259723	-0.5697798	-3.7893749
Fe	9.3914035	1.2792401	-2.8799574
C	10.3593637	-1.7676199	-3.4578151
H	11.4301999	-1.5313063	-3.5190292
H	10.1469042	-2.1390819	-2.4459190
H	10.1564400	-2.5919243	-4.1618776
C	10.7196111	1.3099096	-1.3059149
C	9.3919230	1.5754073	-0.8189897
C	8.9180565	2.7444327	-1.5088558
C	9.9444298	3.1997217	-2.4013317
C	11.0625543	2.3094522	-2.2763066
C	8.6620172	0.8187751	0.2466929
H	8.9782662	-0.2327683	0.2811328
H	8.8712865	1.2559402	1.2370282
H	7.5738736	0.8479853	0.0980625
H	6.7034710	1.3361199	-3.7680207
H	8.6601603	2.2682082	-5.4256023
H	10.7733306	0.5832949	-5.2551814
H	11.3501551	0.4805344	-0.9935700
H	11.9941573	2.3706639	-2.8326209
H	9.8775105	4.0522850	-3.0719510
H	7.9344737	3.1903204	-1.3834195

Model ^{disp}**[c']**$^{+}$:

O	7.2635150	-5.5065831	-1.7371582
C	5.6376533	-1.0284868	-0.6723630
Fe	6.0538556	-2.8752629	-1.0054025
C	7.2292848	-2.0958394	-2.1602444
N	7.9403988	-1.4407790	-2.8438112
C	6.5679130	-4.6174954	-1.4717062
Ni	4.3409481	-4.8040447	-1.4520729
S	4.1354455	-6.2279036	-3.1691170
C	4.1856476	-7.4904057	-1.9638451
N	4.1541666	-8.7904549	-2.2188683
C	4.2139030	-9.7945744	-1.1366663
C	5.6555164	-10.2198555	-0.8594329
N	5.4501462	0.1241019	-0.5570861
S	4.2729839	-6.7809504	-0.3752296
S	4.3240792	-3.6001732	0.4290465
C	2.9748017	-2.3396621	0.3181588
C	2.2089867	-2.3355517	-0.9986381
C	3.0230291	-1.8411695	-2.1879468
S	4.4000169	-2.9584377	-2.7124193
C	4.0703148	-9.3154910	-3.5966801
C	2.6207603	-9.5825908	-4.0013890
C	7.1549384	-2.9080288	0.4095131
O	7.8494241	-2.9242537	1.3273523
H	3.4682672	-0.8580514	-1.9768218
H	2.3862934	-1.7685876	-3.0814376
H	1.8071408	-3.3408702	-1.2064566
H	1.3487828	-1.6541510	-0.8795563
H	2.3043402	-2.6004410	1.1493004
H	3.4313478	-1.3589450	0.5143524
H	3.7451123	-9.3663448	-0.2394142

H	3.5975771	-10.6445789	-1.4643930
H	5.6723415	-10.9879457	-0.0728602
H	6.1213530	-10.6407785	-1.7625947
H	6.2484807	-9.3579569	-0.5221391
H	4.5458835	-8.5906062	-4.2725466
H	4.6697178	-10.2371657	-3.6154883
H	2.5904888	-10.0114408	-5.0133205
H	2.1442445	-10.2953341	-3.3117540
H	2.0447738	-8.6468015	-3.9980481
C	8.3494055	-0.3731842	-3.5973613
C	7.4964980	0.7213427	-3.9840991
C	8.3141061	1.6415549	-4.7144635
C	9.6569886	1.1293032	-4.7386532
C	9.6952848	-0.1233396	-4.0389731
Fe	9.0237712	1.4324584	-2.8032411
C	10.8679450	-1.0248582	-3.8316878
H	11.8033284	-0.4497193	-3.8025362
H	10.7670361	-1.5913046	-2.8947843
H	10.9422843	-1.7507823	-4.6586237
C	10.4317588	1.7540029	-1.2943659
C	9.2219637	1.2483859	-0.7201631
C	8.1616078	2.1515650	-1.0788822
C	8.7278984	3.2215935	-1.8529096
C	10.1355507	2.9699827	-1.9890272
C	9.0620883	-0.0102898	0.0657347
H	9.7950653	-0.7713970	-0.2377214
H	9.2112285	0.1935776	1.1390336
H	8.0448744	-0.4028315	-0.0565625
H	6.4427335	0.8085899	-3.7371353
H	7.9789100	2.5795264	-5.1476399
H	10.5173942	1.6120693	-5.1939707
H	11.4009123	1.2631267	-1.2497382
H	10.8434888	3.5747708	-2.5489297
H	8.1842480	4.0571163	-2.2851773
H	7.1129418	1.9971864	-0.8304644

Model ^{disp}**[c']$^{+}$-H$_2$**:

C	0.0201046	7.4478048	0.1014665
C	0.7995652	6.4798099	0.8121158
C	-0.0731996	5.4534288	1.3015364
C	-1.4045945	5.7873853	0.8740741
C	-1.3508487	7.0212603	0.1393866
Fe	-0.2070798	5.5998737	-0.7830326
C	1.2188723	4.7371642	-2.0591453
C	0.2758358	3.7575054	-1.5846388
C	-1.0633837	4.1530497	-1.9467589
C	-0.9430644	5.3784609	-2.6798940
C	0.4481065	5.7340309	-2.7392061
N	0.5934521	2.6459641	-0.8559623
C	0.6327321	1.6727641	-0.1900464
Fe	0.5570454	0.1761226	0.8698457
C	1.1677726	0.9213303	2.3840851
O	1.5358438	1.3825220	3.3725332
C	2.7007734	4.6820321	-1.8825117
C	0.3222335	4.2392825	2.0743475
C	-1.1354525	0.9688817	1.3326218
N	-2.1266753	1.5492047	1.5703737
C	2.2263594	-0.3254768	0.3757091
O	3.3251911	-0.5027971	0.0718108
Ni	0.2729523	-3.0465019	0.0711080
S	-0.4348133	-1.1111244	-0.8611816
C	-2.2295968	-1.2675120	-0.3816255
C	-2.5040086	-2.1890758	0.8104114

C	-1.7693060	-1.8901922	2.1187277
S	0.0893068	-1.8502101	1.9795883
S	-0.1404859	-4.4040769	-1.7035354
C	0.0643696	-5.7223559	-0.5783118
S	0.3924963	-5.1099859	1.0214540
N	-0.0189146	-7.0086428	-0.8947045
C	-0.2924227	-7.4566216	-2.2748290
C	-1.7887964	-7.6673115	-2.5044090
C	0.1601050	-8.0725922	0.1143030
C	1.6160728	-8.5334911	0.1818875
H	-2.5997521	-0.2503973	-0.2065498
H	-2.7100979	-1.6875000	-1.2766627
H	-2.2896461	-3.2299653	0.5121920
H	-3.5860699	-2.1349249	1.0224070
H	-1.9695436	-2.6985113	2.8362686
H	-2.0746131	-0.9306951	2.5531856
H	-0.1810742	-7.6900434	1.0864613
H	-0.5093231	-8.8952613	-0.1776510
H	1.7147838	-9.3500005	0.9116164
H	1.9575776	-8.9031069	-0.7964256
H	2.2641088	-7.7027552	0.4947986
H	0.1148571	-6.7077272	-2.9686534
H	0.2711157	-8.3903964	-2.4167351
H	-1.9608687	-8.0354241	-3.5260703
H	-2.1947134	-8.4077585	-1.7989670
H	-2.3306852	-6.7199356	-2.3765512
H	3.1299767	5.6928826	-1.8597944
H	2.9667075	4.1610445	-0.9515667
H	3.1652127	4.1348389	-2.7199105
H	1.3349277	3.9091989	1.8016473
H	0.3247489	4.4629783	3.1540684
H	-0.3873657	3.4180456	1.9042612
H	-1.9689842	3.6081068	-1.6976883
H	-1.7669808	5.9490288	-3.0987900
H	0.8597952	6.6283743	-3.1990333
H	1.8812520	6.4875548	0.9234906
H	0.4024776	8.3298230	-0.4052343
H	-2.1911621	7.5290072	-0.3254964
H	-2.2868432	5.1798775	1.0588180
H	2.1677573	-3.0476083	0.1396101
H	2.0335611	-2.8538163	-0.6014111

Model ^{disp}**d**:

C	3.4153435	4.2267793	4.1576071
C	3.6849988	4.7999734	5.4597394
C	5.0510065	5.2611583	5.5068075
C	5.6468716	4.9307621	4.2448253
C	4.6503044	4.2942321	3.4261035
Fe	4.0513956	6.1586159	3.9848183
C	3.8209524	7.2447984	2.2718249
C	4.7686160	7.8852291	3.1450610
C	4.0859527	8.1631840	4.3815198
C	2.7341209	7.6941715	4.2729819
C	2.5696743	7.1219594	2.9670953
C	6.1904571	8.2249865	2.8194407
N	2.7646415	4.9149826	6.4595749
C	2.1180679	4.5524364	7.4018089
Fe	0.7060179	4.6545329	8.6843763
C	-0.4614588	5.0937491	7.4240310
O	-1.2127510	5.3808931	6.5933362
C	2.1146047	3.6366123	3.7227169
Ni	2.5634442	2.6686469	8.3899346
S	3.1069037	1.5258656	6.5237002
C	4.7467377	1.9733997	6.8836822

N	5.7981727	1.7063388	6.1037487
C	7.1816168	1.8819003	6.5733048
C	7.8061671	3.1907228	6.0962151
S	4.8193183	2.8101708	8.4050353
S	2.2700513	3.8076279	10.2873387
C	1.2573166	2.6899120	11.4510624
N	0.7964927	1.4577106	10.8944213
C	-0.2005433	1.5560603	9.8770479
S	0.3588451	2.3251647	8.2237523
C	5.6256018	1.1573055	4.7501982
C	5.6153128	-0.3714881	4.7468574
C	-0.7041787	4.6463353	9.9938185
N	-1.5515297	4.5998738	10.8042710
C	1.1280075	6.3193595	9.1292277
O	1.4050090	7.4048531	9.4136135
H	4.7832240	3.9630250	2.3988655
H	6.6666478	5.1602438	3.9487611
H	1.6697551	6.6436344	2.5894319
H	4.0364946	6.8795123	1.2705923
H	-1.0352891	2.1750812	10.2298027
H	-0.5429304	0.5537204	9.5907854
H	1.5727031	0.8565373	10.6086724
H	1.9470733	2.4898873	12.2806040
H	0.4030810	3.2936681	11.7830420
H	7.1774980	1.8297563	7.6712809
H	7.7507181	1.0158077	6.1985322
H	8.8547121	3.2453839	6.4255406
H	7.7774786	3.2607453	4.9992066
H	7.2529284	4.0442965	6.5084275
H	4.6926933	1.5680191	4.3382811
H	6.4543385	1.5542736	4.1442696
H	5.5178047	-0.7472796	3.7171866
H	6.5486238	-0.7705494	5.1726413
H	4.7680360	-0.7445700	5.3392575
H	1.2743063	4.1620790	4.1990120
H	2.0016688	3.7071234	2.6312906
H	2.0527037	2.5759467	4.0198045
H	4.5371014	8.6145020	5.2616085
H	1.9854276	7.7143812	5.0610666
H	6.6088865	7.5100154	2.0954713
H	6.2620960	9.2338479	2.3776639
H	6.8143728	8.2086236	3.7251570
H	5.5156342	5.7516479	6.3561617

Model $^{disp}\mathbf{d}^{+}$:

C	4.0743120	9.0777139	3.5166314
C	3.4992872	8.8441070	4.8257969
C	2.1973575	8.2327221	4.6781996
C	1.9563969	8.1182435	3.2705007
C	3.0962013	8.6332534	2.5713555
Fe	3.6370694	7.0661329	3.8326213
C	4.3748357	5.4978134	2.6808333
C	3.2753556	5.0385432	3.4784657
C	3.6171089	5.2882432	4.8531776
C	4.9223533	5.8863665	4.8975868
C	5.3885980	6.0193540	3.5475641
C	2.0150811	4.4073432	2.9778716
N	4.1067301	9.1575037	6.0031771
C	4.5287575	9.7480686	6.9464986
Fe	5.4909116	10.1164342	8.5448468
C	6.9923368	9.4490823	7.8271528
O	7.9558010	9.0228198	7.3654831
C	5.4062679	9.6965687	3.2497803
Ni	3.9160436	11.8576649	7.3430121

S	3.9465885	12.6124143	5.2221938
C	2.2357381	12.2637397	5.2089858
N	1.4275976	12.4655012	4.1773785
C	-0.0193748	12.1816323	4.2528954
C	-0.3326320	10.7798724	3.7329042
S	1.7455246	11.6454179	6.7635127
S	3.5986108	11.2149114	9.4586395
C	4.2902430	12.6277590	10.5604701
N	4.9324448	13.6902256	9.8725776
C	6.1709947	13.4132603	9.2388062
S	6.0871920	12.2497153	7.7112465
C	1.9182672	13.0170674	2.8979924
C	1.7877706	14.5392977	2.8637039
C	6.4817201	10.4341026	10.1565211
N	7.0721543	10.6765437	11.1395004
C	4.9108360	8.5825841	9.2772027
O	4.5355965	7.6020660	9.7456084
H	3.2337769	8.6329355	1.4929240
H	1.0746548	7.6771645	2.8139041
H	6.3275522	6.4687776	3.2354225
H	4.4043079	5.4925728	1.5940659
H	6.8583907	12.9157535	9.9350676
H	6.6087254	14.3316117	8.8301537
H	3.4005180	12.9931348	11.0867730
H	4.9893195	12.1354872	11.2485051
H	-0.3430018	12.3003772	5.2966862
H	-0.5222595	12.9555495	3.6549906
H	-1.4162942	10.5990691	3.7743891
H	-0.0011393	10.6648394	2.6898878
H	0.1800443	10.0272717	4.3471445
H	2.9637091	12.7048108	2.7654093
H	1.3209427	12.5435453	2.1049056
H	2.1226726	14.9204677	1.8884134
H	0.7423203	14.8473441	3.0127034
H	2.4071792	14.9930384	3.6498843
H	6.1314811	9.4159729	4.0267932
H	5.7943853	9.3819353	2.2716792
H	5.3227559	10.7955850	3.2591188
H	2.9802455	5.0741849	5.7075314
H	5.4472137	6.2117378	5.7918125
H	1.7712695	4.7554821	1.9643485
H	2.1341799	3.3118122	2.9369345
H	1.1688630	4.6264023	3.6441936
H	1.5400116	7.9428878	5.4920913
H	4.2993613	14.2571746	9.3084451

Model $^{disp}\mathbf{d}^{+}$-$\mathbf{H}_2$:

C	3.1838815	5.3977790	3.2798315
C	3.5555150	5.4739603	4.6675866
C	4.8714523	6.0364958	4.7558098
C	5.3249042	6.3167285	3.4249276
C	4.2869726	5.9193588	2.5172909
Fe	3.5949626	7.3382489	3.8146498
C	3.4923539	9.0460664	4.8954073
C	2.1829991	8.4478266	4.7558403
C	1.9105615	8.3839347	3.3511909
C	3.0423304	8.9131860	2.6407969
C	4.0528791	9.3100954	3.5816089
C	5.3826509	9.9251925	3.2939366
N	4.1198612	9.3088567	6.0765146
C	4.6311234	9.6900064	7.0683942
Ni	3.8107382	12.2448456	7.4870608
S	1.6842586	11.9145100	6.8746449
C	2.2143442	12.2101881	5.2419843
N	1.4420492	12.1656887	4.1650181

C	2.0061856	12.2952658	2.8076990
C	2.0208373	13.7485391	2.3351764
C	1.9041360	4.8485448	2.7309052
Fe	5.5812483	10.0648295	8.6663719
S	3.6421483	11.1577731	9.5184953
C	4.2686754	12.4421364	10.6841583
N	4.9095330	13.5957458	9.9676638
C	6.2256061	13.3313819	9.3007388
S	6.0445697	12.2425830	7.8205616
C	6.5412008	10.4648187	10.2725716
N	7.0923859	10.8023106	11.2517349
C	5.0691721	8.5155464	9.4040645
O	4.7338969	7.5263100	9.8845224
C	7.1010575	9.4140796	7.9837523
O	8.0827869	9.0014807	7.5490981
S	3.9115262	12.5895342	5.2515690
C	-0.0258903	12.0403392	4.2613029
C	-0.4969812	10.5996874	4.0902371
H	3.1535012	8.9540427	1.5601516
H	1.0174906	7.9587775	2.9022542
H	6.2713629	6.7772858	3.1546847
H	4.3061024	6.0262973	1.4357548
H	6.9125449	12.8681561	10.0205745
H	6.5966136	14.3004986	8.9440769
H	5.0045354	14.3926475	10.6125249
H	3.3970643	12.8497797	11.2119807
H	4.9948848	12.0016538	11.3788970
H	-0.3408831	12.4477039	5.2326865
H	-0.4415433	12.6905769	3.4766811
H	-1.5955034	10.5633713	4.1258014
H	-0.1627901	10.1913263	3.1259903
H	-0.0904920	9.9674955	4.8905286
H	3.0156683	11.8598744	2.8198350
H	1.3855239	11.6636359	2.1556121
H	2.4128286	13.8031839	1.3092693
H	1.0058937	14.1732526	2.3368513
H	2.6606307	14.3579609	2.9886384
H	6.1092058	9.6719938	4.0794486
H	5.7714911	9.5667495	2.3309404
H	5.3083346	11.0251429	3.2536470
H	2.9259723	5.1810574	5.5039338
H	5.4118373	6.2562000	5.6730908
H	1.6460742	5.3271980	1.7751199
H	1.9983911	3.7649714	2.5488485
H	1.0745917	4.9996778	3.4364975
H	1.5445751	8.1287660	5.5738394
H	3.5324759	13.7269138	7.9819834
H	4.2160417	13.8377625	9.1259919

Model $^{disp}\mathbf{d}^{+}$**-2H**:

C	3.2465477	5.3205732	3.3569102
C	3.6257434	5.4377330	4.7406748
C	4.9301030	6.0255526	4.8064399
C	5.3679675	6.2884255	3.4698576
C	4.3338624	5.8512402	2.5768302
Fe	3.6021632	7.2877937	3.8385025
C	3.4223762	9.0637145	4.8676551
C	2.1501338	8.3917054	4.7518701
C	1.8812462	8.2585464	3.3512668

C	2.9893646	8.8111957	2.6220218
C	3.9749026	9.2943679	3.5493056
C	5.2778739	9.9546111	3.2427159
N	4.0466448	9.3681736	6.0351680
C	4.5204706	9.8199594	7.0222903
Ni	3.8397512	12.1646382	7.4934718
S	1.6941217	11.7796587	6.8452721
C	2.2259822	12.2094993	5.2441986
N	1.4593298	12.2158305	4.1606805
C	2.0221082	12.4695117	2.8203305
C	1.9957884	13.9550201	2.4624493
C	1.9799765	4.7229532	2.8292570
Fe	5.4884951	10.1154621	8.6218972
S	3.6147270	11.2515427	9.5475068
C	4.3256979	12.5475820	10.6959078
N	4.9617927	13.6366605	9.9814009
C	6.2391128	13.3484407	9.3610576
S	6.0740963	12.2793510	7.8320218
C	6.4879303	10.3864389	10.2338212
N	7.0830686	10.6061602	11.2199358
C	4.9031156	8.5705743	9.3136067
O	4.5233232	7.5806062	9.7590669
C	6.9808733	9.4387215	7.9025024
O	7.9446199	9.0108588	7.4423467
S	3.9108321	12.6502920	5.2759675
C	-0.0056427	12.0456132	4.2369459
C	-0.4367126	10.6062339	3.9722990
H	3.1008165	8.8210163	1.5408242
H	1.0042787	7.7841065	2.9201500
H	6.3019116	6.7654090	3.1851220
H	4.3470198	5.9332061	1.4930681
H	6.9338304	12.8064638	10.0237463
H	6.6836412	14.2894260	9.0129040
H	4.9821391	14.4982882	10.5275122
H	3.4682352	12.9446278	11.2540977
H	5.0124809	12.0045726	11.3656597
H	-0.3390140	12.3822719	5.2287337
H	-0.4329707	12.7322655	3.4906553
H	-1.5345352	10.5417031	3.9746625
H	-0.0674364	10.2603620	2.9959514
H	-0.0375630	9.9405465	4.7485093
H	3.0464122	12.0689653	2.8018322
H	1.4213356	11.8747073	2.1164111
H	2.3898490	14.1023355	1.4465343
H	0.9683904	14.3474552	2.4916198
H	2.6146344	14.5299249	3.1655328
H	6.0161970	9.7494064	4.0309421
H	5.6764569	9.5970130	2.2836745
H	5.1555140	11.0492143	3.1866802
H	3.0093816	5.1500488	5.5885636
H	5.4690578	6.2816636	5.7151145
H	1.7071189	5.1645321	1.8602137
H	2.1047402	3.6375657	2.6803724
H	1.1487249	4.8714190	3.5332073
H	1.5276366	8.0761827	5.5832940
H	3.8341967	13.8524495	8.4731731
H	3.3754641	13.8835724	7.8083439

Model $^{disp}\mathbf{d}_{TS}^{+}$**-H$_2$**:

C	4.0049631	9.0258841	3.4948736
C	3.4082507	8.8792982	4.8096688
C	2.1344790	8.2020295	4.6963084
C	1.9195034	7.9726542	3.2979625
C	3.0523199	8.4765987	2.5715646
Fe	3.6348259	7.0652966	3.9309459

C	4.4865535	5.5647402	2.8316248
C	3.3637585	5.0556573	3.5730810
C	3.6349663	5.2924836	4.9662064
C	4.9104141	5.9364837	5.0780152
C	5.4384922	6.1100688	3.7568091
C	2.1617983	4.3677759	3.0058256
N	4.0088247	9.2593133	5.9702706
C	4.5471178	9.6641642	6.9391591
Fe	5.5337701	9.9878530	8.5310947
C	7.0290216	9.3108093	7.8231193
O	7.9950363	8.8827196	7.3680700
C	5.3088891	9.6909290	3.1988942
Ni	3.8065617	12.1351384	7.3806556
S	3.8680004	12.7402193	5.2127627
C	2.1638039	12.3842967	5.1818159
N	1.3582009	12.5924730	4.1493707
C	-0.0756689	12.2506434	4.1998332
C	-0.3304293	10.8669457	3.6041843
S	1.6809444	11.7635933	6.7350191
S	3.6268587	11.1088807	9.4071839
C	4.2815441	12.4143341	10.5461062
N	4.9093818	13.5374842	9.7985223
C	6.2287291	13.2512757	9.1719036
S	6.0634344	12.1502679	7.6916411
C	1.8478519	13.2026470	2.8971499
C	1.7205610	14.7256446	2.9395903
C	6.5124656	10.3516476	10.1354265
N	7.0741498	10.6774976	11.1123796
C	4.9892592	8.4402353	9.2443768
O	4.6339462	7.4481282	9.7052581
H	3.1998554	8.4098501	1.4967612
H	1.0615852	7.4631601	2.8676537
H	6.3762333	6.5952746	3.5001360
H	4.5751478	5.5631133	1.7482917
H	6.8994790	12.7745099	9.8994856
H	6.6326639	14.2061390	8.8127875
H	4.9769996	14.3683509	10.3999663
H	3.4192518	12.8246305	11.0867989
H	5.0101610	11.9599542	11.2310423
H	-0.4080383	12.3025624	5.2467932
H	-0.6069256	13.0358287	3.6418138
H	-1.4035476	10.6323527	3.6518485
H	-0.0150677	10.8296416	2.5508978
H	0.2300709	10.1024307	4.1606365
H	2.8926729	12.8948697	2.7454554
H	1.2501925	12.7694513	2.0822130
H	2.0559521	15.1562992	1.9851355
H	0.6757127	15.0273420	3.1053931
H	2.3410171	15.1374107	3.7479681
H	6.0351485	9.5040716	4.0034446
H	5.7300287	9.3151268	2.2564945
H	5.1801166	10.7833918	3.1142613
H	2.9669096	5.0456763	5.7872466
H	5.3725881	6.2796239	6.0000162
H	1.9463381	4.7223914	1.9876985
H	2.3343216	3.2796022	2.9532011
H	1.2754867	4.5363815	3.6340989
H	1.4817585	7.9395778	5.5230376
H	3.5301095	13.6411790	7.9166154
H	4.1602315	13.7136871	8.8460705

Model ^{disp}**e**:

C	5.5028978	4.8204055	4.8139873
C	4.4722347	4.3800465	3.9081734
C	3.1981110	4.6466043	4.5262250
C	3.4685726	5.2089685	5.8280078
C	4.8901580	5.3519482	5.9971457

Fe	4.2622535	6.3605329	4.3478888
C	3.2287945	8.1213450	4.3644866
C	3.1927958	7.5238835	3.0595364
C	4.5474597	7.3788362	2.6030026
C	5.4296177	7.8810996	3.6225469
C	4.6048200	8.3418598	4.7087905
H	2.3004402	7.1974958	2.5316198
C	6.9252250	7.9379981	3.5584500
C	1.8234890	4.3733794	4.0073050
N	1.2653974	3.1339803	4.5566978
C	-0.1506957	3.0200350	4.2208219
N	2.4940799	5.5513841	6.7215880
C	1.8006461	5.3125984	7.6736848
Ni	2.2483534	3.6794142	9.0013027
S	4.4792729	3.9587189	9.2578607
C	4.6327303	2.8402919	7.9336685
N	5.7882154	2.4716177	7.3673432
C	7.0949152	2.7945421	7.9577888
C	7.8280499	3.9119022	7.2162732
C	2.0065067	1.9737014	4.0805918
Fe	0.2532155	5.5341444	8.7704327
C	-1.2979437	5.6370170	9.9037972
N	-2.2307062	5.6691742	10.6150356
S	0.0992728	3.1403710	8.6813597
C	-0.6243739	2.6119385	10.2994063
C	0.3173579	2.7387006	11.4920474
C	0.6404734	4.1785136	11.8749277
S	1.6704104	5.0884666	10.6381521
S	3.0710942	2.2873478	7.4290019
C	0.5170194	7.2804798	8.9399205
O	0.6901586	8.4192778	9.0365664
C	-0.7734076	5.6376967	7.3324272
O	-1.4286140	5.6918409	6.3800726
C	5.8008969	1.6422734	6.1529081
C	5.7707292	0.1481991	6.4770051
C	4.6774956	3.7463850	2.5691631
H	6.5704959	4.7969549	4.6096444
H	4.8628027	6.9242921	1.6667276
H	-1.5362649	3.2054513	10.4575787
H	-0.8938203	1.5570871	10.1431311
H	1.2517731	2.1865364	11.2917221
H	-0.1745668	2.2637465	12.3596882
H	1.2409936	4.1994975	12.7959696
H	-0.2810222	4.7600380	12.0219201
H	6.9347883	3.0672279	9.0101344
H	7.6879730	1.8655109	7.9392530
H	8.8304846	4.0482713	7.6490738
H	7.9426017	3.6687225	6.1496552
H	7.2750899	4.8560331	7.2991976
H	4.9374161	1.9383726	5.5387055
H	6.7094921	1.9120355	5.5942897
H	5.8144230	-0.4424992	5.5498250
H	6.6294462	-0.1318287	7.1064011
H	4.8437590	-0.1023422	7.0115897
H	1.8431208	4.3512819	2.8912658
H	4.9709374	8.7463613	5.6490472
H	2.3719850	8.3173567	5.0034391
H	7.3215112	7.1357779	2.9185101
H	7.2646627	8.9021598	3.1422173
H	7.3646861	7.8318573	4.5615449
H	5.3684837	5.7701677	6.8757262
H	1.1619218	5.1995983	4.3114742
H	1.5880596	1.0614890	4.5298926
H	1.9649605	1.8789050	2.9690466
H	3.0590665	2.0588271	4.3875511
H	-0.5626989	2.1117866	4.6844755
H	-0.6949821	3.8906022	4.6145007
H	-0.3199472	2.9614439	3.1193202
H	4.7115987	2.6459484	2.6535426
H	3.8513050	3.9975409	1.8881256
H	5.6201644	4.0858098	2.1152325

Model $^{disp}\mathbf{e}^{+}$:

C	5.6867818	5.3909522	4.3111785
C	4.6170388	4.8345821	3.5259803
C	3.4438146	4.7832194	4.3505426
C	3.8187359	5.2710818	5.6559545
C	5.2015359	5.6826526	5.6301621
Fe	4.1360966	6.7250709	4.2434932
C	2.7197930	8.1876458	4.4726405
C	2.7974857	7.7936544	3.0964999
C	4.1322409	8.0454841	2.6430183
C	4.8927326	8.5956956	3.7274047
C	4.0133854	8.6752209	4.8629819
H	1.9959746	7.3487639	2.5130064
C	6.3272258	9.0163837	3.6859856
C	2.0722907	4.2901758	4.0168948
N	1.8156908	2.9804216	4.6252650
C	0.4063310	2.6134524	4.5214951
N	2.9554321	5.3630465	6.6957876
C	2.1412187	5.2008251	7.5465650
Ni	2.2619737	3.5315176	8.9856357
S	4.5225262	3.6015965	9.2090918
C	4.5234447	2.2972884	8.0552356
N	5.6077953	1.7035699	7.5702506
C	6.9656108	2.1118952	7.9777838
C	7.5556348	3.1130086	6.9848132
C	2.6837765	1.9454342	4.0756052
Fe	0.5956840	5.5658274	8.6068616
C	-0.9546916	5.9655467	9.6569863
N	-1.8910995	6.1706508	10.3316339
S	0.0706485	3.2592522	8.6267032
C	-0.7506517	2.9016580	10.2439205
C	0.1711127	2.9601657	11.4561613
C	0.6775198	4.3586494	11.7894118
S	1.8516406	5.0748034	10.5547999
S	2.8869176	1.8759887	7.6211060
C	1.0631495	7.2902929	8.7412149
O	1.3632654	8.3985373	8.8181362
C	-0.3828589	5.7380065	7.1233742
O	-0.9974924	5.8314564	6.1522011
C	5.5179359	0.5907456	6.6038100
C	5.4415606	-0.7597523	7.3154669
C	4.6979603	4.3950052	2.0992965
H	6.6919708	5.5900390	3.9480806
H	4.5261965	7.8124292	1.6567702
H	-1.5791319	3.6182739	10.3414582
H	-1.1538872	1.8867202	10.1189192
H	1.0206302	2.2698708	11.3215530
H	-0.4069701	2.6040002	12.3261996
H	1.2544280	4.3428081	12.7250092
H	-0.1559624	5.0699871	11.8826290
H	6.9112028	2.5397383	8.9886172
H	7.5697362	1.1944581	8.0323337
H	8.5654838	3.4074820	7.3045310
H	7.6253430	2.6741806	5.9782304
H	6.9217054	4.0092706	6.9333473
H	4.6364275	0.7579947	5.9683017
H	6.4118591	0.6588985	5.9665541
H	5.4165855	-1.5724005	6.5750078
H	6.3169728	-0.9119686	7.9639477
H	4.5316425	-0.8151497	7.9291915
H	1.9458578	4.2620575	2.9108822
H	4.2939147	9.0290479	5.8516216
H	1.8464923	8.1025554	5.1141403
H	6.8842050	8.4528491	2.9243815
H	6.3993352	10.0872181	3.4323402
H	6.8118142	8.8714153	4.6619576
H	5.7482773	6.1136975	6.4630463
H	1.3258246	4.9930010	4.4174714
H	2.4882801	0.9970846	4.5960459
H	2.5144826	1.7937621	2.9859009

H	3.7369673	2.2231533	4.2321617
H	0.2381050	1.6697033	5.0595722
H	-0.2142685	3.3965231	4.9804649
H	0.0828832	2.4788297	3.4658464
H	4.9253562	3.3173709	2.0400467
H	3.7429397	4.5608018	1.5809291
H	5.4882527	4.9392610	1.5645833

Model ^{disp}**e**$^{+}$**-2H**:

C	3.9778101	9.6473381	4.3430117
C	2.9794024	9.8691459	5.3533782
C	1.6993931	9.9599874	4.6863315
C	1.9433964	9.7995241	3.2620144
C	3.3517663	9.5903305	3.0553682
Fe	2.5567995	8.1791894	4.2952780
C	1.5702446	6.5461124	3.5398676
C	1.2648548	6.7228800	4.9296653
C	2.4973088	6.6629330	5.6637215
C	3.5729822	6.4496978	4.7334433
C	2.9885222	6.3785892	3.4201284
C	5.0233294	6.2998804	5.0706351
C	0.3649814	10.1419477	5.3032566
N	-0.0965650	11.5938262	5.3316349
C	0.8845955	12.5012029	5.9884268
N	0.9607758	9.8600316	2.3147435
C	-0.0609045	10.1140219	1.7708310
Fe	-1.6484214	10.2810093	0.8254576
C	-3.2733313	10.3634016	-0.1975389
N	-4.2648102	10.3994993	-0.8217838
C	-0.9353081	9.5018993	-0.6233928
O	-0.4818379	9.0118863	-1.5599579
C	-2.3133199	8.7886700	1.5537859
O	-2.7494513	7.8434871	2.0494258
S	-0.9613383	12.4423078	0.1395928
Ni	-0.9327811	13.1823032	2.3132649
S	-1.5404839	14.6688439	3.9984240
C	-0.2603688	15.6635380	3.3397917
N	0.0255970	16.8940948	3.7576759
C	1.0963639	17.6981696	3.1348804
C	2.4194584	17.5376743	3.8828661
S	-2.5665635	11.6685478	2.5184451
C	-3.9415821	12.6246828	1.6970650
C	-3.4598736	13.7153439	0.7353528
C	-2.5267284	13.2921021	-0.4034174
S	0.5535896	14.8473744	2.0352404
C	-0.7383217	17.5552544	4.8343252
C	-1.9032109	18.3681647	4.2693218
C	-1.4494422	11.6971299	5.9488366
C	3.2203278	10.0054461	6.8239073
H	5.0358601	9.4915998	4.5369243
H	0.2758462	6.8901729	5.3490046
H	2.6122624	6.7878494	6.7376489
H	-4.5796703	11.8863958	1.1962077
H	-4.4879908	13.0909286	2.5291600
H	-2.9735112	14.5145806	1.3218723
H	-4.3591623	14.1594425	0.2752565
H	-2.1800251	14.1899244	-0.9346637
H	-3.0261843	12.6169020	-1.1081770
H	1.1946679	17.3914449	2.0840540
H	0.7526109	18.7430670	3.1485845
H	3.1877893	18.1768998	3.4244883
H	2.3119964	17.8322306	4.9375447
H	2.7598474	16.4933784	3.8353258
H	-1.0979167	16.7834498	5.5289637

H	-0.0262431	18.1960745	5.3749988
H	-2.4297595	18.8842230	5.0850773
H	-1.5453083	19.1264258	3.5571326
H	-2.6131245	17.7049033	3.7557170
H	0.1318259	12.2925709	2.9883143
H	-0.4093019	9.6020919	4.7408346
H	0.3621065	9.7954617	6.3464775
H	3.5420474	6.2564454	2.4929157
H	0.8585827	6.5787641	2.7191605
H	5.2803377	6.8709356	5.9746819
H	5.2653120	5.2411574	5.2621536
H	5.6597515	6.6449765	4.2430907
H	3.8300725	9.4150439	2.0967814
H	0.5013386	13.5243439	5.8885471
H	0.9819058	12.2151314	7.0439783
H	1.8462602	12.3995435	5.4730620
H	-1.7493859	12.7510641	5.9455959
H	-2.1522599	11.1092198	5.3462588
H	-1.3938830	11.3135652	6.9766794
H	-0.1541251	11.9267805	4.2987541
H	3.4185565	11.0549039	7.1016737
H	2.3524844	9.6580712	7.4055572
H	4.0915323	9.4096056	7.1296313

Model ^{solv}**c**:

C	3.5477028	4.7148032	3.7144048
C	3.8000612	5.0649999	5.0790454
C	5.0757544	5.7190414	5.1521632
C	5.6479113	5.7941517	3.8373308
C	4.7023879	5.1363317	2.9523021
Fe	3.8121945	6.7392773	3.8922058
C	2.0780822	7.6467102	3.2371790
C	3.2011834	8.1066825	2.4725572
C	4.1383062	8.7060461	3.3783085
C	3.5858058	8.6182128	4.7007681
C	2.3063121	7.9623287	4.6236813
C	1.3555195	7.7287836	5.7596229
C	6.9982425	6.3145092	3.4580639
N	4.8838025	4.9439126	1.6165284
C	5.1327047	4.5854718	0.5055083
Fe	5.1490788	4.8647076	-1.4233814
C	5.2006009	5.0880391	-3.3320162
N	5.2146025	5.2639677	-4.4941494
C	3.4501152	5.3643051	-1.4098549
O	2.3388535	5.6897466	-1.4128375
C	5.8259388	6.4875538	-1.2203617
O	6.2726413	7.5491348	-1.0995750
S	7.3373402	3.9184162	-1.3717554
Ni	6.0520628	2.6937221	0.0024564
S	7.5979107	2.4707719	1.6275490
C	6.4737051	1.3773422	2.3866181
N	6.7030322	0.7006756	3.5096987
C	5.6904553	-0.2105067	4.0809351
C	4.8340377	0.4607083	5.1544558
S	4.5006260	2.5750546	-1.6119381
C	5.2765505	1.8934740	-3.1555520
C	6.7874981	1.7031442	-3.0959579
C	7.5917316	2.9904039	-2.9602660
S	5.0206146	1.2806542	1.4288179
C	7.9896863	0.8206692	4.2265300

C	8.9988014	-0.2497345	3.8084117
H	5.5318028	6.1248808	6.0520655
H	3.1239186	4.8895967	5.9114855
H	5.1024765	9.1324650	3.1138379
H	4.0612740	8.9653990	5.6154817
H	7.3685396	3.6904180	-3.7760678
H	8.6676468	2.7689169	-2.9664781
H	7.0458786	1.0124691	-2.2775169
H	7.0975997	1.2156415	-4.0370619
H	4.7766872	0.9253862	-3.2961358
H	4.9896038	2.5631765	-3.9772094
H	5.0658879	-0.5772788	3.2549807
H	6.2316837	-1.0742970	4.4919060
H	4.1110494	-0.2658200	5.5514867
H	5.4471207	0.8209902	5.9925121
H	4.2772238	1.3102349	4.7370176
H	8.3878523	1.8268138	4.0355383
H	7.7653233	0.7537851	5.2998812
H	9.9256121	-0.1223430	4.3853368
H	8.6159519	-1.2616011	4.0016596
H	9.2423318	-0.1633525	2.7408667
H	6.9959493	6.7512334	2.4501980
H	7.3327813	7.0849957	4.1653953
H	7.7430161	5.5014644	3.4641171
H	1.2065370	7.1288739	2.8429125
H	3.3320273	7.9937418	1.3993033
H	1.8904044	7.5946414	6.7101304
H	0.6792699	8.5918533	5.8797523
H	0.7314875	6.8417239	5.5850554
H	2.6762923	4.2078319	3.3109696

Model $^{solv}\mathbf{c}^{+}$:

C	3.7969304	4.7940663	3.9104110
C	4.1792665	5.1545232	5.2407202
C	5.4600096	5.8011018	5.1794360
C	5.9052274	5.8403281	3.8156909
C	4.8843571	5.1693216	3.0415471
Fe	4.0505425	6.8663477	4.1055122
C	2.8820036	8.1833196	2.9156642
C	4.1417266	8.7656098	3.2736037
C	4.1959634	8.8347058	4.7068847
C	2.9715008	8.2860414	5.2153272
C	2.1445133	7.8964959	4.1082871
C	0.7696098	7.3165863	4.1891262
C	7.2031347	6.3649745	3.2973363
N	4.9077872	5.0137186	1.6991637
C	5.0728100	4.5927546	0.5830573
Fe	4.9613829	4.7880779	-1.3249176
C	4.8750853	4.9767430	-3.2393183
N	4.8070912	5.1255040	-4.4019304
C	3.2555912	5.2915707	-1.2336577
O	2.1493837	5.6182517	-1.1879676
C	5.6581683	6.4236632	-1.2323619
O	6.1096494	7.4848092	-1.1789473
S	7.1517909	3.8564258	-1.4295640
Ni	5.9078583	2.7406150	0.0807433
S	7.5470512	2.5422309	1.6154963

C	6.4707905	1.4495996	2.4493843
N	6.7757142	0.7553345	3.5375568
C	5.8020420	-0.1664722	4.1633322
C	5.0231807	0.4863181	5.3046076
S	4.2707092	2.5106292	-1.4405020
C	4.9568883	1.7783639	-3.0000581
C	6.4664192	1.5788317	-3.0220721
C	7.2805076	2.8661530	-2.9923814
S	4.9511074	1.3723172	1.5950319
C	8.1164417	0.8471606	4.1573301
C	9.0654484	-0.2453914	3.6646420
H	6.0128030	6.2046558	6.0238949
H	3.5929533	4.9773326	6.1379035
H	5.0183424	9.2224234	5.3019793
H	2.7134308	8.1672574	6.2649098
H	7.0030399	3.5384010	-3.8149984
H	8.3534024	2.6418511	-3.0632323
H	6.7730073	0.9176690	-2.1962905
H	6.7150488	1.0541764	-3.9606495
H	4.4407448	0.8116443	-3.0741343
H	4.6228167	2.4231223	-3.8240646
H	5.1230366	-0.5226634	3.3766654
H	6.3724490	-1.0341937	4.5217511
H	4.3393058	-0.2526540	5.7447041
H	5.6935350	0.8421342	6.0991805
H	4.4248564	1.3325318	4.9408166
H	8.5211279	1.8449081	3.9381238
H	7.9691854	0.7837586	5.2439762
H	10.0349908	-0.1361307	4.1700394
H	8.6778187	-1.2483233	3.8904982
H	9.2295740	-0.1658362	2.5817201
H	7.1002148	6.7915455	2.2910681
H	7.6130319	7.1321600	3.9655382
H	7.9355803	5.5441074	3.2334153
H	2.5433256	7.9686238	1.9046645
H	4.9140383	9.0982910	2.5855307
H	0.6313269	6.7270907	5.1042850
H	0.0329940	8.1364797	4.2092663
H	0.5411530	6.6885830	3.3187857
H	2.8842660	4.2957771	3.5973561

Model $^{solv}\mathbf{c}^{+}$-$\mathbf{H_2}$:

C	3.1729529	9.6758473	3.3379934
C	3.9581880	9.4430590	4.5078427
C	3.0768553	9.3888249	5.6406786
C	1.7271779	9.6009086	5.2010889
C	1.8058874	9.7882909	3.7709251
Fe	2.5946607	7.9045232	4.2799974
C	3.3125577	6.2360059	3.2092660
C	1.9023366	6.3866590	3.0318325
C	1.2840572	6.3132352	4.3247185
C	2.3257964	6.1198970	5.2936858
C	3.5882700	6.0605076	4.6055374
C	4.9281985	5.8241953	5.2269446
C	0.4989067	9.6962099	6.0462591
N	0.7383094	10.0447061	2.9551940
C	-0.1749592	10.3431236	2.2666015
Fe	-1.6473561	10.5015870	1.1306379
C	-3.1666879	10.4413620	-0.0523715
N	-4.0804769	10.3071680	-0.7767255
C	-0.8047001	9.5255573	-0.1137625
O	-0.2645369	8.9164172	-0.9294853

C	-2.4549034	9.1551125	1.9925564
O	-2.9927564	8.3001123	2.5479044
S	-2.6317115	12.1509212	2.5283000
Ni	-0.9763124	13.6582539	2.1690413
S	-1.4903503	15.1321606	3.8281279
C	-0.4377389	16.2477299	2.9928199
N	-0.1944789	17.4946153	3.3736203
C	0.7227379	18.3695433	2.6092016
C	2.1536041	18.3272437	3.1455269
S	-0.8568910	12.5393130	0.2038990
C	-2.3451570	13.3376907	-0.5882596
C	-3.3625852	13.9179462	0.3949502
C	-3.9218596	12.9902960	1.4746168
S	0.2369796	15.4878320	1.5733203
C	-0.8351765	18.0745153	4.5751633
C	-2.1117508	18.8461977	4.2418184
H	3.3724397	9.2147811	6.6720486
H	5.0366149	9.3138322	4.5287850
H	0.2211444	6.3934395	4.5362173
H	2.1912122	6.0386165	6.3697414
H	-4.5529035	12.1951074	1.0624683
H	-4.5116809	13.5774529	2.1911862
H	-2.9195938	14.8025217	0.8820698
H	-4.2177241	14.2888447	-0.1960613
H	-1.9200988	14.1485612	-1.1950275
H	-2.7830630	12.5873918	-1.2553908
H	0.6871545	18.0569008	1.5569586
H	0.3093408	19.3858064	2.6647017
H	2.7796218	19.0123469	2.5572370
H	2.1997099	18.6438238	4.1967012
H	2.5767268	17.3168343	3.0624353
H	-1.0425267	17.2536338	5.2746052
H	-0.0890587	18.7288729	5.0465419
H	-2.5299566	19.2689077	5.1658340
H	-1.9125211	19.6757477	3.5495469
H	-2.8659243	18.1858952	3.7929767
H	0.6906677	12.9059057	2.8301895
H	0.2321825	12.8658419	3.4532261
H	-0.3984698	9.3720914	5.5032309
H	0.5972665	9.0851310	6.9520247
H	0.3409555	10.7392955	6.3639499
H	4.0608905	6.2892288	2.4218255
H	1.3958892	6.5524585	2.0844139
H	4.9765050	6.2239972	6.2481946
H	5.1207046	4.7405460	5.2860131
H	5.7347120	6.2709810	4.6310265
H	3.5216640	9.7602915	2.3128678

Model ^{solv}**c'**:

O	7.1163636	-4.8894105	-1.3347703
C	4.7472357	-0.8312749	-0.0001153
Fe	5.4903777	-2.5274614	-0.5278671
C	6.6370441	-1.6163666	-1.6445590
N	7.3579652	-1.0242018	-2.3664818
C	6.2364382	-4.1595034	-1.0879495
Ni	4.1814910	-4.7346017	-1.3217599
S	4.3494990	-5.9489765	-3.2126447
C	4.4248222	-7.3416263	-2.1659960
N	4.5464382	-8.6019920	-2.5719260
C	4.6095219	-9.7182174	-1.6048918
C	6.0448103	-10.1028397	-1.2442362

N	4.3238762	0.2150602	0.3270066
S	4.2980112	-6.8290525	-0.5045864
S	3.8341537	-3.7509082	0.6631360
C	2.2525573	-2.7795113	0.6245556
C	1.5533444	-2.7242544	-0.7276502
C	2.3224252	-1.9710773	-1.8054862
S	3.9253924	-2.7461162	-2.3314740
C	4.6224477	-8.9437393	-4.0078232
C	3.2580450	-9.2924737	-4.6033927
C	6.5401985	-2.4794250	0.8893638
O	7.2160199	-2.4394459	1.8302756
H	2.5567159	-0.9471177	-1.4840233
H	1.7357141	-1.9269370	-2.7329863
H	1.3187118	-3.7437241	-1.0730383
H	0.5896049	-2.2049334	-0.5829876
H	1.6166092	-3.2860434	1.3630966
H	2.4898335	-1.7717819	0.9914708
H	4.0473317	-9.4198888	-0.7094063
H	4.0767881	-10.5648159	-2.0595235
H	6.0290102	-10.9493420	-0.5434177
H	6.6156885	-10.4090520	-2.1320832
H	6.5666431	-9.2653773	-0.7618436
H	5.0718393	-8.0894691	-4.5322152
H	5.3192516	-9.7885821	-4.0975504
H	3.3806842	-9.5580365	-5.6628323
H	2.8016957	-10.1501976	-4.0898684
H	2.5714383	-8.4376918	-4.5390941
C	8.1379908	-0.3452008	-3.2655281
C	7.7249598	0.8163965	-4.0197365
C	8.7994147	1.1344410	-4.9104627
C	9.8628786	0.1946355	-4.6941831
C	9.4782578	-0.7314367	-3.6665151
Fe	9.4289088	1.2062929	-2.9531402
C	10.2355944	-1.9310428	-3.1903975
H	11.3179489	-1.7747993	-3.2888797
H	10.0155727	-2.1583095	-2.1386120
H	9.9693527	-2.8199383	-3.7861509
C	10.7474549	1.3132919	-1.3736033
C	9.4311211	1.6891947	-0.9295052
C	9.0204563	2.8137199	-1.7278733
C	10.0755793	3.1331688	-2.6471681
C	11.1469739	2.2022059	-2.4278148
C	8.6584129	1.0649538	0.1914588
H	8.9362735	0.0112368	0.3299311
H	8.8663405	1.5880270	1.1395948
H	7.5749343	1.1167827	0.0166868
H	6.7693949	1.3245404	-3.9267975
H	8.8149735	1.9661647	-5.6100664
H	10.8235969	0.1933018	-5.2037887
H	11.3304334	0.4818156	-0.9838536
H	12.0830144	2.1623638	-2.9792616
H	10.0564166	3.9226523	-3.3946219
H	8.0608926	3.3205021	-1.6556628

Model ^{solv}**[c']**$^{+}$:

O	7.1367627	-4.8851007	-1.4361735
C	4.7030835	-0.8841335	-0.0554520
Fe	5.4502403	-2.5748375	-0.5916110
C	6.5780507	-1.6302984	-1.6767154
N	7.2976308	-1.0036321	-2.3739908
C	6.2522241	-4.1772273	-1.1644375

Ni	4.1776596	-4.7601341	-1.3405191
S	4.2887776	-5.9721949	-3.2259138
C	4.4210729	-7.3649297	-2.1793833
N	4.5543320	-8.6180341	-2.5873736
C	4.6631666	-9.7353220	-1.6222832
C	6.1145572	-10.0964614	-1.3067947
N	4.2814937	0.1619520	0.2703424
S	4.3325029	-6.8474655	-0.5148846
S	3.8351450	-3.7845919	0.6500408
C	2.2380858	-2.8417301	0.6119291
C	1.5298193	-2.8072292	-0.7354707
C	2.2717242	-2.0435125	-1.8242964
S	3.8838425	-2.7850870	-2.3665160
C	4.6029702	-8.9599747	-4.0269074
C	3.2336127	-9.3469620	-4.5854880
C	6.5001312	-2.5331806	0.8505262
O	7.1691028	-2.4917182	1.7896742
H	2.4893548	-1.0121445	-1.5154216
H	1.6785667	-2.0202110	-2.7481641
H	1.3079407	-3.8313913	-1.0737197
H	0.5591332	-2.3044054	-0.5844132
H	1.6203634	-3.3596879	1.3577070
H	2.4615192	-1.8302098	0.9770783
H	4.1214179	-9.4470639	-0.7110187
H	4.1304835	-10.5877350	-2.0651043
H	6.1305352	-10.9481027	-0.6126427
H	6.6642752	-10.3882019	-2.2124615
H	6.6369523	-9.2549599	-0.8322299
H	5.0171719	-8.0952631	-4.5628824
H	5.3201697	-9.7856126	-4.1303013
H	3.3397916	-9.6069469	-5.6478277
H	2.8158974	-10.2191706	-4.0639559
H	2.5234323	-8.5132543	-4.5034048
C	8.0760829	-0.3356569	-3.2747886
C	7.7160009	0.8879039	-3.9430481
C	8.7938092	1.2047080	-4.8300580
C	9.8124200	0.2049341	-4.6739440
C	9.3837823	-0.7618770	-3.7067768
Fe	9.4785972	1.2169975	-2.8884765
C	10.0967708	-2.0032709	-3.2838730
H	11.1817333	-1.8935041	-3.4007667
H	9.8790641	-2.2655447	-2.2406574
H	9.7750678	-2.8473188	-3.9149670
C	10.7263606	1.2610199	-1.1976653
C	9.4836495	1.8811314	-0.8405264
C	9.2777425	2.9700194	-1.7499431
C	10.3995640	3.0443460	-2.6402274
C	11.3010041	1.9798760	-2.2972168
C	8.5740055	1.4695741	0.2713676
H	8.6983531	0.4085537	0.5228706
H	8.8163227	2.0515646	1.1752844
H	7.5203424	1.6628213	0.0312308
H	6.7861059	1.4331518	-3.8103930
H	8.8341883	2.0620514	-5.4958215
H	10.7649676	0.1780336	-5.1965844
H	11.1523083	0.3834272	-0.7172732
H	12.2421834	1.7518367	-2.7900992
H	10.5340082	3.7667140	-3.4408766
H	8.4057589	3.6192277	-1.7678362

Model ^{solv}**[c']$^{+}$-H$_2$**:

C	0.2562092	7.6225147	-0.3364860
C	0.8101583	6.7347788	0.6412154
C	-0.2456876	5.9428178	1.1993317
C	-1.4605561	6.3333572	0.5392534
C	-1.1576844	7.3774851	-0.3987817
Fe	-0.1311932	5.6755016	-0.9178699

C	1.2952230	4.4788675	-1.9673226
C	0.2282313	3.6652238	-1.4394190
C	-1.0374733	4.1268284	-1.9497949
C	-0.7514713	5.2206654	-2.8265754
C	0.6680574	5.4393055	-2.8254354
N	0.3934289	2.6003010	-0.5966288
C	0.4480009	1.6349592	0.0789824
Fe	0.4594943	0.1092441	1.1136950
C	1.1883761	0.8026886	2.5937603
O	1.6340159	1.2340546	3.5658204
C	2.7564488	4.2965345	-1.7180420
C	-0.1127512	4.9121124	2.2740516
C	-1.1998983	0.8127318	1.8039218
N	-2.1614181	1.3338549	2.2300073
C	2.0957861	-0.3110249	0.4655814
O	3.1770935	-0.4213006	0.0768983
Ni	0.1770594	-3.1099956	0.1510933
S	-0.6444852	-1.1362020	-0.5890862
C	-2.3892659	-1.3858130	0.0236110
C	-2.5311412	-2.3883097	1.1689125
C	-1.6939592	-2.1527066	2.4258639
S	0.1412024	-2.0065924	2.1254510
S	-0.2759456	-4.3659261	-1.6854441
C	0.0659942	-5.7482801	-0.6753756
S	0.4620999	-5.2244246	0.9428284
N	0.0279792	-7.0115874	-1.0782643
C	-0.3320651	-7.3679103	-2.4686306
C	-1.8197366	-7.6813243	-2.6280175
C	0.3438188	-8.1257808	-0.1573691
C	1.8086186	-8.5560198	-0.2400668
H	-2.7752931	-0.3939648	0.2837408
H	-2.9291248	-1.7584701	-0.8573284
H	-2.3164467	-3.3993357	0.7840015
H	-3.5918716	-2.3932331	1.4741194
H	-1.7855726	-3.0196057	3.0938688
H	-1.9957978	-1.2517779	2.9714492
H	0.0851961	-7.8046683	0.8605515
H	-0.3271643	-8.9546090	-0.4216963
H	1.9765293	-9.3981032	0.4455312
H	2.0758790	-8.8865056	-1.2535382
H	2.4776208	-7.7350485	0.0510989
H	-0.0342226	-6.5329294	-3.1170669
H	0.2853149	-8.2343615	-2.7425011
H	-2.0198890	-7.9602496	-3.6718803
H	-2.1263254	-8.5209042	-1.9887158
H	-2.4361552	-6.8065105	-2.3808645
H	3.2995605	5.2398515	-1.8530709
H	2.9553107	3.9189559	-0.7063459
H	3.1676921	3.5666639	-2.4340323
H	0.9030073	4.4977715	2.3097230
H	-0.3148044	5.3737725	3.2542213
H	-0.8319412	4.0917190	2.1453331
H	-2.0086773	3.6975277	-1.7222416
H	-1.4864463	5.7919248	-3.3864155
H	1.1938074	6.2130163	-3.3790471
H	1.8629482	6.6513110	0.9015329
H	0.8100225	8.3392053	-0.9369584
H	-1.8687555	7.8804541	-1.0486848
H	-2.4427302	5.9026397	0.7191267
H	2.2024113	-3.1295063	0.0175525
H	2.0210388	-2.8608151	-0.6799049

Model ^{solv}**d**:

C	3.5877600	4.7087327	3.8330537
C	3.7661946	5.1005678	5.2197873
C	5.0456560	5.7573454	5.3712663
C	5.6818327	5.7282059	4.0893323
C	4.7959300	5.0908763	3.1570224
Fe	3.9000194	6.7442547	3.9876304
C	3.4019545	7.9821197	2.4212771
C	4.3597149	8.6364367	3.2748649
C	3.7696292	8.7161084	4.5859833
C	2.4659787	8.1205974	4.5385358
C	2.2371377	7.6626794	3.1979876
C	5.6859837	9.1995386	2.8590122
N	2.8698919	4.8745409	6.2208248
C	2.2293611	4.4742266	7.1450431
Fe	0.7947610	4.6228002	8.4489343
C	-0.3876805	4.9923690	7.1833422
O	-1.1725113	5.2287972	6.3654413
C	2.4315896	3.9430332	3.2719384
Ni	2.6607525	2.6169727	8.1838541
S	3.1537301	1.2313562	6.4771473
C	4.8239728	1.4885626	6.9028470
N	5.8638630	0.8972566	6.3194294
C	7.2495856	1.1691406	6.7532649
C	7.9348402	2.2386385	5.9019307
S	4.9133685	2.6102439	8.2341589
S	2.3871799	3.8335288	10.0472979
C	1.4223816	2.7549112	11.3009150
N	0.9199286	1.5089894	10.8200769
C	-0.0811195	1.5553900	9.8044556
S	0.4422653	2.2838639	8.1117855
C	5.6756445	-0.0725261	5.2206220
C	5.5973042	-1.5171860	5.7163686
C	-0.5962654	4.7210441	9.7742564
N	-1.4568411	4.8175656	10.5691733
C	1.2328745	6.3013503	8.8030446
O	1.5088327	7.3988940	9.0480608
H	4.9877654	4.9412378	2.0970007
H	6.6588582	6.1447985	3.8587372
H	1.3486260	7.1495113	2.8383042
H	3.5507640	7.7490514	1.3692608
H	-0.9321397	2.1645905	10.1304889
H	-0.4072242	0.5409314	9.5506489
H	1.6665318	0.8465426	10.6010096
H	2.1526961	2.5833038	12.0990570
H	0.6025246	3.3893607	11.6570871
H	7.2170310	1.4715760	7.8088437
H	7.7942366	0.2162121	6.7013156
H	8.9634102	2.3852150	6.2606780
H	7.9844846	1.9424262	4.8446776
H	7.4026244	3.1966208	5.9726535
H	4.7594674	0.2044447	4.6811485
H	6.5180478	0.0614496	4.5282244
H	5.4789082	-2.1914363	4.8564855
H	6.5113528	-1.8092124	6.2524983
H	4.7373356	-1.6565140	6.3850449
H	1.4870978	4.2218912	3.7584434
H	2.3293848	4.1239334	2.1936139
H	2.5737332	2.8603546	3.4234180
H	4.2461487	9.1388269	5.4676166
H	1.7849837	8.0072176	5.3778972
H	6.1222389	8.6284230	2.0280753
H	5.5729922	10.2432014	2.5208784
H	6.4019862	9.1986105	3.6927124
H	5.4399820	6.1643812	6.2975308

Model $^{solv}\mathbf{d}^{+}$:

C	4.3169245	8.7837333	3.3509928
C	3.6572507	8.6989654	4.6326941
C	2.3894044	8.0189153	4.4762471
C	2.2427977	7.7372782	3.0794717
C	3.4234586	8.1905852	2.4043701
Fe	3.8717222	6.7337789	3.8427819
C	4.5280280	4.9843261	2.8403346
C	3.4444495	4.6731457	3.7291392
C	3.8660103	5.0625068	5.0529717
C	5.2026750	5.5818865	4.9675418
C	5.6047156	5.5357589	3.5982219
C	2.1554067	4.0075417	3.3651827
N	4.1710932	9.1526678	5.8038806
C	4.4826668	9.8018604	6.7623377
Fe	5.4372099	10.0818690	8.4077410
C	6.9392455	9.4561370	7.6794186
O	7.9188941	9.0536283	7.2217356
C	5.6348157	9.4281994	3.0781789
Ni	3.8250674	11.7879477	7.1874773
S	3.8184875	12.7216244	5.1372090
C	2.0858620	12.5060039	5.1785560
N	1.2369424	12.9268894	4.2513950
C	-0.2207780	12.7102334	4.3861094
C	-0.6958390	11.4460603	3.6701313
S	1.6423280	11.6938431	6.6584464
S	3.5149553	11.1477426	9.3144240
C	4.1426840	12.5646210	10.4538166
N	4.7811655	13.6604612	9.8142435
C	6.0208167	13.4194628	9.1640540
S	5.9750074	12.2657669	7.6251437
C	1.7056782	13.6555042	3.0512405
C	1.6452149	15.1725047	3.2279322
C	6.4208529	10.3482980	10.0425289
N	7.0363296	10.4770527	11.0339106
C	4.8520764	8.5245990	9.0490751
O	4.4751170	7.5196007	9.4718723
H	3.6276174	8.0875884	1.3414852
H	1.3879317	7.2519303	2.6166134
H	6.5474116	5.8975298	3.1956589
H	4.5134853	4.8567672	1.7603449
H	6.7369164	12.9463823	9.8459643
H	6.4280280	14.3498249	8.7548918
H	3.2260400	12.8931201	10.9547069
H	4.8199978	12.0734649	11.1617386
H	-0.4565010	12.6676302	5.4581236
H	-0.7119943	13.6032221	3.9769943
H	-1.7852302	11.3561855	3.7819665
H	-0.4674577	11.4798790	2.5958651
H	-0.2318228	10.5494035	4.1027386
H	2.7313563	13.3263678	2.8367282
H	1.0732072	13.3283689	2.2147450
H	1.9838883	15.6568279	2.3015827
H	0.6215642	15.5144240	3.4340140
H	2.2984034	15.5003191	4.0476097
H	6.3451155	9.2748927	3.9011466
H	6.0786316	9.0421310	2.1526220
H	5.4975189	10.5153621	2.9597209
H	3.2747189	4.9581639	5.9589750
H	5.7975714	5.9626573	5.7939000
H	1.8674569	4.2245487	2.3285382
H	2.2696932	2.9151964	3.4563063
H	1.3396059	4.3109371	4.0340270
H	1.6773941	7.8191679	5.2711860
H	4.1419783	14.2377221	9.2658711

Model ^{solv}**d^{+}-2H**:

C	3.4301909	4.8415044	3.6020401
C	3.6991167	5.1026376	4.9923793
C	4.9993884	5.6963551	5.1014588
C	5.5464567	5.8154965	3.7814159
C	4.5805260	5.2886597	2.8598583
Fe	3.7756350	6.8630975	3.9134442
C	3.5876013	8.7281278	4.7256161
C	2.2943725	8.0873583	4.6206661
C	2.0841550	7.8194176	3.2317043
C	3.2362748	8.2621295	2.5000123
C	4.1970600	8.8190330	3.4091912
C	5.4952278	9.4813993	3.0737581
N	4.1445500	9.1988763	5.8812650
C	4.5958892	9.6824684	6.8587831
Ni	3.7429496	12.2633720	7.3587335
S	1.6003352	12.0060744	6.7599580
C	2.0676696	12.6042458	5.1896060
N	1.2392358	12.8620527	4.1864172
C	1.7339015	13.4151973	2.9066723
C	1.6437169	14.9401752	2.8541108
C	2.2181365	4.1606724	3.0417080
Fe	5.5386092	10.0532393	8.4753053
S	3.6124563	11.1272809	9.3537578
C	4.2258854	12.3818873	10.5611149
N	4.8733478	13.5544388	9.8935257
C	6.1732292	13.3108908	9.1973396
S	5.9786836	12.2525943	7.6962619
C	6.5218044	10.3611962	10.0937293
N	7.1325544	10.5374336	11.0811058
C	5.0098618	8.4893633	9.1568875
O	4.6635160	7.4879529	9.6089150
C	7.0517097	9.4290440	7.7621057
O	8.0366943	9.0308751	7.3159505
S	3.7923438	12.8483017	5.1693587
C	-0.2147407	12.6191829	4.3055952
C	-0.6346415	11.2688910	3.7252853
H	3.3817703	8.1664137	1.4267715
H	1.2093240	7.3325407	2.8089941
H	6.5109109	6.2447318	3.5226359
H	4.6846435	5.2531292	1.7778545
H	6.8809666	12.8461892	9.8914887
H	6.5391177	14.2841189	8.8541461
H	4.9858086	14.3195205	10.5743637
H	3.3481985	12.7646656	11.0925187
H	4.9343005	11.9206312	11.2563449
H	-0.4798204	12.6901841	5.3696444
H	-0.7186566	13.4459663	3.7869283
H	-1.7224769	11.1543825	3.8294536
H	-0.3877171	11.1934722	2.6572404
H	-0.1475447	10.4413296	4.2581122
H	2.7718176	13.0795774	2.7741975
H	1.1353270	12.9558630	2.1084045
H	2.0014619	15.2889920	1.8755558
H	0.6086354	15.2873488	2.9789566
H	2.2662243	15.3995581	3.6335287
H	6.2434892	9.3384626	3.8653450
H	5.9065228	9.0796049	2.1388994
H	5.3542519	10.5667822	2.9417186
H	3.0193095	4.8969387	5.8157675
H	5.4748415	6.0257689	6.0219224
H	2.0143102	4.4859201	2.0124316
H	2.3693362	3.0686679	3.0207109
H	1.3269271	4.3593348	3.6524305
H	1.6190696	7.8822611	5.4459137
H	3.4466924	13.7288841	7.8841691
H	4.1876120	13.8656653	9.1177658

Model ^{solv}**e**:

C	5.5355541	5.6395104	4.2217951
C	4.5479447	5.1179350	3.3136288
C	3.3198566	4.9259392	4.0511830
C	3.5942924	5.3104687	5.4261685
C	4.9568983	5.7787063	5.5215841
Fe	3.9094845	6.8926956	4.1529873
C	2.4414446	8.3130544	4.4475963
C	2.5636727	8.0042517	3.0524070
C	3.9072367	8.3090555	2.6510506
C	4.6274631	8.8068159	3.7930901
C	3.7107948	8.8028668	4.9040530
H	1.7833831	7.5909855	2.4181206
C	6.0422515	9.3027582	3.8102167
C	2.0111488	4.3797306	3.5559226
N	1.7768138	2.9823729	3.9544466
C	0.4114615	2.5781624	3.6294528
N	2.7058820	5.2624202	6.4560150
C	2.0569166	5.1006212	7.4440057
Ni	2.4123556	3.5923424	8.9366827
S	4.6602503	3.5901083	9.1342256
C	4.6143540	2.1147927	8.2043448
N	5.6640231	1.3378803	7.9404228
C	7.0214383	1.6863725	8.4049916
C	7.8481615	2.3964817	7.3321340
C	2.7479747	2.0657689	3.3656369
Fe	0.5721326	5.6018376	8.6135285
C	-0.8850063	6.0354827	9.7904297
N	-1.7897760	6.3374668	10.4775907
S	0.1902687	3.2597619	8.8357099
C	-0.4534862	2.9478924	10.5491245
C	0.5651773	3.1232289	11.6688502
C	1.0737070	4.5477843	11.8532882
S	2.0644626	5.2247660	10.4357079
S	2.9795371	1.7915405	7.7100903
C	1.0478705	7.3063294	8.5754520
O	1.3510941	8.4241550	8.5680316
C	-0.5294615	5.6828744	7.2312659
O	-1.2609859	5.7423433	6.3349331
C	5.5063928	0.0732327	7.1935730
C	5.2734764	-1.1280088	8.1117915
C	4.7880741	4.7920734	1.8698590
H	6.5534881	5.9117886	3.9516058
H	4.3245547	8.1638346	1.6569884
H	-1.3197284	3.6086573	10.6894971
H	-0.8041287	1.9074361	10.5141507
H	1.4150756	2.4395426	11.5125629
H	0.0785433	2.8193907	12.6123612
H	1.7652694	4.5980445	12.7053019
H	0.2464922	5.2492193	12.0271940
H	6.9178897	2.3168407	9.2983027
H	7.5043268	0.7499500	8.7181056
H	8.8503257	2.6133851	7.7279627
H	7.9653698	1.7730015	6.4349930
H	7.3793697	3.3460819	7.0402247
H	4.6671515	0.1982668	6.4954241
H	6.4166686	-0.0608645	6.5933328
H	5.1801016	-2.0396514	7.5048379
H	6.1106700	-1.2698607	8.8098015
H	4.3489422	-1.0031178	8.6912598
H	1.9605859	4.5034610	2.4493774
H	3.9518246	9.1048940	5.9204988
H	1.5517045	8.1734960	5.0563328
H	6.6504659	8.8071105	3.0413546
H	6.0733138	10.3871568	3.6112866
H	6.5154188	9.1331224	4.7873885
H	5.4341713	6.1472433	6.4245611
H	1.1881040	4.9763859	3.9776400
H	2.5576317	1.0470532	3.7324124

H	2.7035293	2.0461732	2.2518777
H	3.7645659	2.3514631	3.6661704
H	0.2346874	1.5557545	3.9924196
H	-0.3056042	3.2473106	4.1255266
H	0.2011681	2.5957959	2.5350847
H	5.1088813	3.7433858	1.7537787
H	3.8830290	4.9286377	1.2630513
H	5.5797259	5.4291904	1.4523739

Model $^{solv}\mathbf{e}^{+}$:

C	5.5246638	5.7194584	4.1126596
C	4.5252408	5.1548208	3.2482128
C	3.3343460	4.9377285	4.0260014
C	3.6357993	5.3427093	5.3816591
C	4.9836936	5.8640184	5.4299686
Fe	3.8933501	6.9886143	4.0987142
C	2.3841171	8.3827603	4.3471809
C	2.5528867	8.1192558	2.9497163
C	3.8879430	8.4823343	2.5923758
C	4.5616660	8.9797374	3.7554926
C	3.6274016	8.9014666	4.8480332
H	1.8065785	7.6941348	2.2836500
C	5.9564130	9.5152808	3.8172784
C	2.0198564	4.3670266	3.5743116
N	1.8343625	2.9727090	4.0044069
C	0.4591737	2.5309662	3.7785568
N	2.7792875	5.2844028	6.4297160
C	2.1061038	5.1351729	7.4048127
Ni	2.4364553	3.5854105	8.8730298
S	4.6858275	3.5809629	9.0702150
C	4.6188579	2.0745993	8.1899119
N	5.6423443	1.2547524	7.9925068
C	6.9998473	1.5757669	8.4857687
C	7.8827653	2.2012339	7.4057390
C	2.8000973	2.0555181	3.4038187
Fe	0.6434167	5.5992974	8.5868398
C	-0.8080686	6.0362866	9.7637720
N	-1.7032490	6.3279298	10.4654476
S	0.2093159	3.2747791	8.7574579
C	-0.4298059	2.9203204	10.4627955
C	0.5899232	3.0591571	11.5858277
C	1.1094616	4.4734650	11.8093475
S	2.1033393	5.1883162	10.4142269
S	2.9803286	1.7759265	7.6662127
C	1.1271512	7.3125285	8.5948430
O	1.4325707	8.4259896	8.6160859
C	-0.4830108	5.7279832	7.2158679
O	-1.2274314	5.8216762	6.3375250
C	5.4641156	-0.0429967	7.3032371
C	5.1965247	-1.1903145	8.2783335
C	4.7194504	4.8306377	1.7997903
H	6.5301652	6.0015519	3.8099067
H	4.3362687	8.3655346	1.6082642
H	-1.2933381	3.5812888	10.6169662
H	-0.7843984	1.8832392	10.3945861
H	1.4317968	2.3682605	11.4199698
H	0.0965734	2.7390113	12.5196272
H	1.8068189	4.4949951	12.6575210
H	0.2910248	5.1791518	12.0047474
H	6.8934114	2.2497151	9.3462127
H	7.4337806	0.6367176	8.8549823
H	8.8818509	2.3902453	7.8221111
H	7.9971809	1.5342122	6.5404024

H	7.4676317	3.1580914	7.0615591
H	4.6356758	0.0656384	6.5900057
H	6.3784119	-0.2222271	6.7220588
H	5.0943028	-2.1272854	7.7135273
H	6.0223941	-1.3144767	8.9925376
H	4.2674598	-1.0211452	8.8387329
H	1.9369395	4.4714793	2.4700320
H	3.8348872	9.1980213	5.8730381
H	1.4778052	8.2131907	4.9224171
H	6.5959729	9.0686226	3.0451320
H	5.9376207	10.6036820	3.6442181
H	6.4127112	9.3458202	4.8012888
H	5.4854633	6.2419493	6.3156425
H	1.1984777	4.9539670	4.0107435
H	2.6375280	1.0463058	3.8052275
H	2.7110061	2.0064914	2.2965017
H	3.8235543	2.3612463	3.6579224
H	0.3332339	1.5173192	4.1825930
H	-0.2400336	3.2005904	4.2974989
H	0.1862938	2.5097967	2.7012769
H	5.0580429	3.7877883	1.6913076
H	3.7915725	4.9386711	1.2239998
H	5.4869223	5.4751543	1.3525247

Model $^{solv}\mathbf{e}^{+}$**-2H**:

C	3.9881134	9.5081219	4.1314374
C	3.1435616	9.7807707	5.2614757
C	1.7870066	9.9142345	4.7707150
C	1.8387378	9.7207792	3.3266893
C	3.2004670	9.4580840	2.9388722
Fe	2.5190479	8.0674797	4.2834243
C	1.5215041	6.4158212	3.5403521
C	1.1940278	6.6202772	4.9211211
C	2.4129039	6.5495184	5.6768401
C	3.5012872	6.2994058	4.7701245
C	2.9378789	6.2233553	3.4476442
C	4.9372215	6.0818084	5.1397383
C	0.5480851	10.1951336	5.5466912
N	0.1223264	11.6676062	5.5378191
C	1.1748938	12.5853651	6.0706068
N	0.7600564	9.8312760	2.4919269
C	-0.2194913	10.1138816	1.8939078
Fe	-1.7327162	10.2899562	0.8010684
C	-3.2308393	10.3575857	-0.4053036
N	-4.1276300	10.3205045	-1.1623005
C	-0.8833792	9.4203503	-0.5075589
O	-0.3433244	8.8696631	-1.3651253
C	-2.5097329	8.8654073	1.5481553
O	-3.0302706	7.9613105	2.0422122
S	-0.9011232	12.4089971	0.1302589
Ni	-1.0788561	13.2549951	2.2721296
S	-1.7824976	14.7500551	3.8933952
C	-0.4539841	15.7378309	3.3370924
N	-0.1667295	16.9517487	3.7958724
C	0.9762525	17.7276468	3.2665431
C	2.2377303	17.5699006	4.1162009
S	-2.7739506	11.7844270	2.3349299
C	-4.0075718	12.7624380	1.3314825
C	-3.3871319	13.8001852	0.3944162
C	-2.3522244	13.3076630	-0.6181000

S	0.4286616	14.9144012	2.0758888
C	-0.9977588	17.6033503	4.8324710
C	-2.0994440	18.4789747	4.2346917
C	-1.1764097	11.8360616	6.2641736
C	3.6115170	9.9492337	6.6756035
H	5.0596193	9.3312286	4.1821441
H	0.2009461	6.8029652	5.3241486
H	2.5050382	6.6765399	6.7530036
H	-4.6257888	12.0324088	0.7968620
H	-4.6238478	13.2705823	2.0853939
H	-2.9379622	14.6045805	1.0016338
H	-4.2113127	14.2674325	-0.1712550
H	-1.9028258	14.1690248	-1.1300807
H	-2.7878826	12.6367571	-1.3669546
H	1.1550101	17.4016075	2.2330357
H	0.6560209	18.7778773	3.2286096
H	3.0383712	18.1921328	3.6928007
H	2.0695981	17.8941441	5.1527006
H	2.5812730	16.5265619	4.1235037
H	-1.4260047	16.8149842	5.4660729
H	-0.3163199	18.1972696	5.4562994
H	-2.6644878	18.9549179	5.0481327
H	-1.6840875	19.2748031	3.6006940
H	-2.7966552	17.8784232	3.6353155
H	-0.1176648	12.3544392	3.1045836
H	-0.3113482	9.6473159	5.1391914
H	0.6621846	9.9180312	6.6021431
H	3.5015205	6.0712454	2.5303078
H	0.8258588	6.4354917	2.7052158
H	5.2111069	6.6430900	6.0434022
H	5.1171609	5.0140290	5.3472709
H	5.6129637	6.3788230	4.3263462
H	3.5458927	9.2681286	1.9270220
H	0.8081611	13.6136749	5.9870603
H	1.3630166	12.3395282	7.1217025
H	2.0865895	12.4645314	5.4777350
H	-1.4868864	12.8829807	6.1821778
H	-1.9284920	11.1865271	5.8031815
H	-1.0322582	11.5611085	7.3148915
H	-0.0427936	11.9544376	4.5162842
H	3.8830069	10.9984334	6.8767983
H	2.8440388	9.6560075	7.4048774
H	4.5050228	9.3393693	6.8627377