Supporting Information

Electric-Field Effects on the [FeFe]-Hydrogenase Active Site

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1 QM calculations

All-electron calculations were performed with density functional theory (BP86 exchange-correlation functional[1,2] and def2-TZVP basis set[3] on all atoms) as implemented in the TURBOMOLE program package.[4] Partial charges were obtained from Mulliken population analysis. The resolution of the identity approximation (RI)[5] was invoked for the SCF procedure and dispersion corrections were considered by Grimme's DFT-D3[6] correction.

The structures were taken from Ref.,[7] but they were optimized as isolated systems (without embedding into a dielectric continuum as electric field effects are explicitly considered in this work) with certain atoms anchored to model the structural constraints exerted by the protein environment. In addition to the H-cluster, the model contains backbone atoms of residues 232, 324 and 325, side chain atoms of residue Ser232 and atoms of truncated side chains of Cys299, Ser323, Lys358 and Glu361 (labeling according to pdb entry 3C8Y). The hydrogen atoms representing the link to the protein, where the model is truncated, and the corresponding carbon atoms of the QM model were kept frozen during structure optimization. In addition, the backbone C, O and N atoms of residues 232, 324 and 325 were kept frozen. This procedure ensures that the position and direction constraints of the protein are maintained. The antiferromagnetic coupling pattern was adjusted such that the two iron atoms most distant from the $[2Fe]_H$ subcluster constitute one ferromagnetically coupled layer and the two iron atoms of the cubane closest to the $[2Fe]_H$ subcluster form the second ferromagnetically coupled layer. If there is spin density in the $[2Fe]_H$

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subcluster it was chosen to couple antiferromagnetically to the closest layer of the cubane. This coupling pattern has also been described by Fiedler and Brunold.[8] The wave function was converged to an energy threshold of 10^{-7} hartree. The geometric gradient was converged to 10^{-4} hartree in the structure optimizations.

The effect of the RI approximation was tested for $[FeFe]_{Ox}$ and field $\vec{E}^{0}_{prot}$. The difference in partial charges was found to not exceed 0.007 e and the difference in the sum of partial charges over the parts did not exceed 0.001 e. Hence, it has no effect on our interpretation.

The effect of the field of the protein on structure optimizations was tested. The structural changes are small and the reaction energies are not significantly affected (see Table 1), which is the reason why all results reported in the letter have been obtained for the field-free BP86-D3/def2-TZVP structures.

Table 1: Effect of structure optimizations on the electronic energy. ΔE are the difference in electronic energy for the starting structure (obtained in a field-free constrained structure optimization) and the converged structure with field $\vec{E}^{0}_{prot}$ in kcal/mol.

Intermediate	ΔE [kcal/mol]	structural change
$[FeFe]_{Ox}$	−1.67	small
$[FeFe]_{Red}$	−3.19	medium
$[FeFe]^{H^+}$	−1.94	small
$[FeFe] - H^-$	−1.57	small
$[FeFe]^{\mu} - H^-$	−1.58	small
$[FeFe]^{H^+} - H^-$	−1.25	small
$[FeFe] - H_2$	−1.15	small
$[FeFe]_{Red} - H_2$	−1.55	small
$[FeFe]_{Ox} - O_2$	−1.51	small
$[FeFe]_{Red} - O_2$	−2.50	small–moderate
$[FeFe]^{\mu}_{Ox}$	−2.49	moderate
$[FeFe]^{\mu}_{Red}$	−2.76	small–moderate

2 DelPhi calculation

2.1 Methodology

The field within a protein can be obtained. as the derivative of the electrostatic potential. A reliable method to calculate the electrostatic potential of whole proteins is the numerical solution of the (nonlinear) Poisson-Boltzmann equation on a grid.[9,10] We took advantage of the DelPhi program[11] for solving the Poisson-Boltzmann equation based on a crystal structure of the [FeFe] hydrogenase from *Clostridium pasteurianum* (pdb code: 3C8Y).[12] The PARSE set of

partial charges, which is optimized for electrostatic potential calculations, was applied.[13] The crystal structure was protonated with the REDUCE program[14] and protonation states where checked with PROPKA.[15] There are no charges available for the atoms of iron-sulfur cubanes within the PARSE set. Therefore, their charge was set to zero and the charges of the coordinating cysteine residues were adapted so that the total charge resembles the charge of the cluster in its normal oxidation state (−2 for [4Fe-4S], −2 for [2Fe-2S]).[16] Since we are interested in the field created from the protein around the H-cluster, charges on the H-cluster were set to zero as well. Note that the crystal-water molecules have been removed, and their effect is considered by a dielectric continuum which fills cavities in the protein (and surrounds the protein structure).

2.2 Crystal structure from *Clostridium pasteurianum* (pdb code: 3C8Y)

A list of assignments of protonation states of histidine residues is given in Table 2. There is no radius defined for iron in the PARSE set. However, the radii are Pauling radii from Ref.[17] In Ref.[17] it is stated that Pauling radii are approximately the covalent radii +0.8 Å. The covalent radius of Fe(II) is approximately 1.2 Å,[17] and hence, the radius for iron was chosen to be 2 Å.

There are no charges available for the three additional [4Fe-4S] cluster and the [2Fe-2S] available in the PARSE set. Because the normal oxidation state 2Fe(III)2Fe(II) corresponds to a total charge of −2 (including coordinated cysteinates) for the [4Fe-4S] clusters, a charge of zero was assigned to two cysteinate ligands and the charge of all [4Fe-4S] atoms was set to zero. Thus, a total charge of −2 is obtained. The charge on the cysteinate ligands was adjusted by changing the partial charges on the sulfur and C_β atoms to give a total charge of zero. The same procedure was applied to the [2Fe-2S] cluster which was assumed to be in the oxidized state Fe(III)Fe(III) (charge −2). Cysteinates with charge changed to zero are residues: 34, 49, 98, 107, 150, 200, 157, 196.

Our goal was to calculate the field generated from the protein matrix around the H-cluster. Thus, the H-cluster was considered as uncharged in the potential calculation. In addition the, partial charges of the side chains of residues Lys358 and Glu361, which are involved in the salt bridge to the CN^- ligand at Fe_d were set to zero; they are contained in the QM model.

Additional parameters set in DelPhi: salt=0.1, scale=3.0, perfil=50, bndcon=4, relpar=1.2, indi=2.0, exdi=80.0, prbrad=1.4, rmsc=0.0001.

The field vectors around Fe_d are presented in Figure 1. The field vectors above Fe_d corresponds to the field at the position of the bound hydride. The dispersion of the field vectors is small. Only the field at the carbon atom of the cyanide ligand significantly deviates from the other field vectors. This is because the cyanide ligand is involved in hydrogen bonds and already close to the backbone atoms which carry partial charges. Close to charged atoms the potential varies strongly and thus the field vectors become strongly position dependent. However, around Fe_d (including Fe_p) the field vectors are similar. This supports the assumption to choose the field at Fe_d as homogeneous field

Table 2: List of assigned protonation states of histidine residues for the potential calculation. δ indicates a proton at N_δ and ϵ indicates a proton at N_ϵ

residue	protonation state
His94	δ
His210	δ and ϵ
His224	δ and ϵ
His492	δ and ϵ
His500	δ and ϵ
His511	δ and ϵ
His536	δ and ϵ
His543	δ and ϵ
His565	δ and ϵ
His569	δ and ϵ

in the QM calculations — apart from the natural assumption that the electric and electronic situation at Fe_d determines the coordination chemistry at Fe_d — and the scanning of the field strength ensures that the effects due to variation of the field are covered.

2.3 Comparison to the [FeFe] hydrogenase from *Desulfovibrio desulfuricans* (pdb code: 1HFE)

The [FeFe] hydrogenase from *Desulfovibrio desulfuricans* (HydDd) is structurally different compared to the [FeFe] hydrogenase from *Clostridium pasteurianum* (HydCp). It does not have an [2Fe-2S] cluster and the sequence identity is only 30%. However, the coordination sphere around the H cluster is similar.

The electric field of a monomer of the dimeric crystal structure was calculated as described above. The H-cluster was considered as uncharged and the partial charges of the side chains of residues Lys237 and Glu240 (labeling according to pdb: 1HFE, L strain) The assignments of the protonation states of the histidine residues is given in Table 4. A single cysteine molecule present in the crystal structure was assigned to be in the zwitterionic state and the partial charges were adapted accordingly. The resulting electric field at Fe_d is shown in Figure 2.

The field has a direction similar to the field obtained for HydCp. It is tilted away from the cubane and has a strength of 0.0026 a.u. which is approximately two third of the field obtained for HydCp. Comparing the low sequence identity of the two [FeFe] hydrogenases it is remarkable that the field at Fe_d is that similar. From the calculation for HydCp we observed that with increasing field strength the hydride and H_2 formation steps become less endothermic.

The specific activities of both enzymes are listed in Table 3.[18] When comparing the activities for the as isolated species it appears that HydDd has a lower activity for H_2 oxidation than HydCp and a higher activity for H_2 formation. This trend is, however, not clear if the activated form of HydDd is

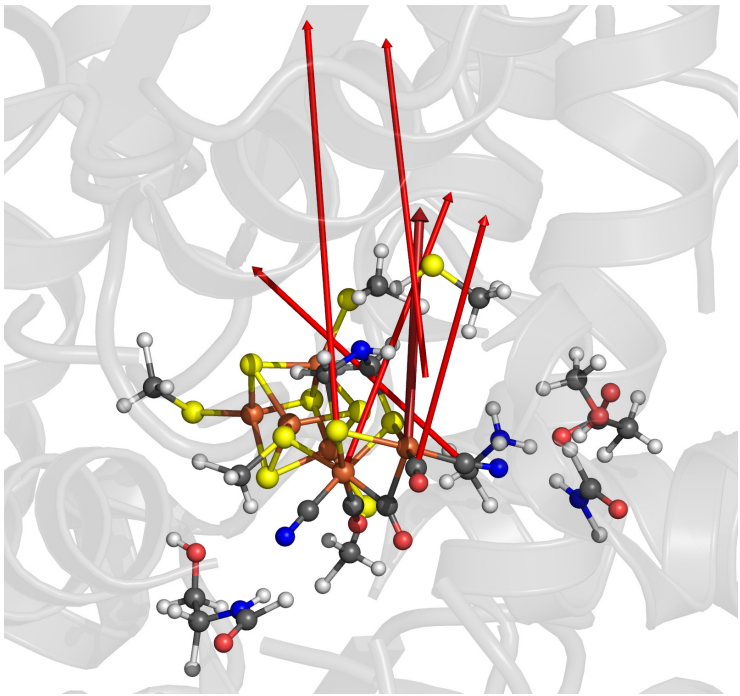

Figure 1: The electric field vectors of the potential calculation around Fe_d are plotted as red arrows. The shown atoms belong to the QM model.

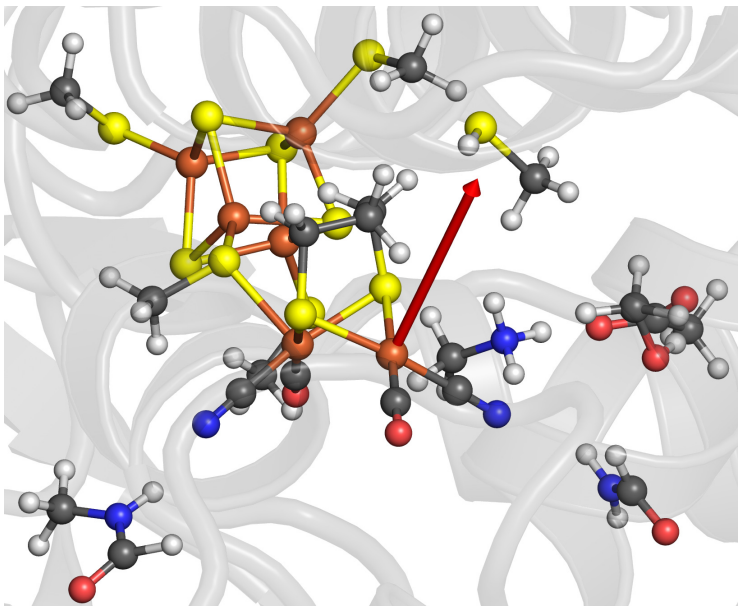

Figure 2: H-cluster and selected atoms of surrounding amino acids from the crystal structure of [FeFe] hydrogenase from *Desulfovibrio desulfuricans* (pdb code: 1HFE). Backbone atoms of residues Pro108, Ala109, Pro203 and Ile204, side chain atoms of residues Cys178, Glu240, Lys237 and Ser202 are shown (labeling according to 1HFE, L strain). These atoms correspond to those selected for the QM region of the structure from *Clostridium pasteurianum* (pdb code: 3C8Y). The field vector of the protein at Fe_d is shown in red.

considered since the H_2 oxidation activity increases upon activation (activated data for HydCp not available). For H_2 formation the activity is, according to Table 3, always higher for HydDd than for HydCp, which is in line with our expectations. Note, however, that the external conditions are not the same for the presented literature values.

Table 3: Specific activities of [FeFe]-Hydrogenases taken from the literature as cited in the Table. Activities are for species as isolated and activated, if available, in brackets.

	H_2 oxidation (U)	H_2 formation (U)
Desulfovibrio desulfuricans aerobic purification [19]	19300 (62200)	8200 (8200)
Clostridium pasteurianum I anaerobic purification [20]	24000	5500
Clostridium pasteurianum II anaerobic purification [20]	34000	10

Table 4: List of assigned protonation states of histidine residues for the potential calculation. δ indicates a proton at N_δ and ϵ indicates a proton at N_ϵ

residue	strand	protonation state
His14	L	δ
His26	L	ϵ
His58	L	ϵ
His62	L	ϵ
His75	L	δ
His141	L	δ
His196	L	δ
His351	L	ϵ
His371	L	ϵ
His14	M	δ
His26	M	ϵ
His58	M	ϵ
His62	M	ϵ
His75	M	δ
His196	M	δ
His371	M	ϵ
His82	S	δ
His85	S	ϵ
His89	S	ϵ
His91	S	ϵ
His82	T	δ
His85	T	ϵ
His89	T	ϵ
His91	T	ϵ

3 μ-Hydride species

The hydride species can be terminally bound to Fe_d or in a μ-bridging fashion between Fe_d and Fe_p. The μ-bridging hydride species in thermodynamically more stable but its formation is kinetically hindered. In this section the effect of the field on two possible μ-hydride formation pathways is investigated. The μ-hydride species can be formed by isomerization of the terminal hydride species or it is suggested that the Fe–Fe bond could be directly protonated with the ammonium group of Lys358 (labeling according to pdb code: 3C8Y) as proton source.[7,21] The two reactions are depicted in Figure 3.

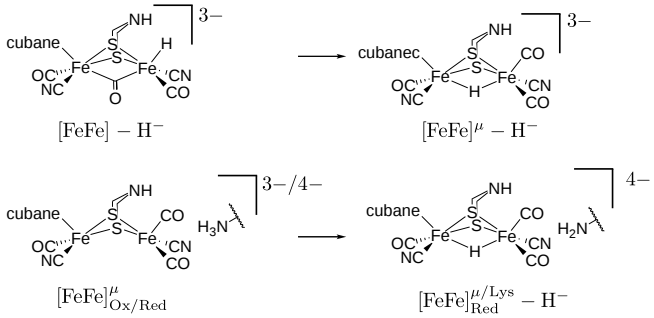

Figure 3: The two possible μ-hydride formation pathways. The superscript "μ" indicates the conformation with an empty coordination site in the μ-bridging position. The superscript "Lys" indicates that Lys 358 is the proton source.

The reaction energies for the different field strengths are shown in Table 5. Isomerization of the terminal hydride species to the μ-bridging hydride species is energetically not affected by the fields in direction of $\vec{E}^{0}_{\text{prot}}$. However, $\vec{E}_{\text{Fe-Fe}}$ results in a +4.6 kcal/mol less exothermic reaction. Inversion of the field $-\vec{E}_{\text{Fe-Fe}}$ results in a −2.5 kcal/mol more exothermic reaction. Notably, the stabilities of the terminal and μ-hydride isomers basically remain unchanged. Also, if Lys 358 serves as proton source, the hydride formation reaction is not affected.

Table 5: Reaction energies in kcal/mol for the μ-hydride formation for the different electric field strengths calculated with BP86-D3/def2-TZVP (single-points on BP86-D3/in-vacuo structures; no dielectric continuum model applied). The field strengths in a.u. are: $|\vec{E}^{-3}_{\text{prot}}| = 0.0008$, $|\vec{E}^{-2}_{\text{prot}}| = 0.0018$, $|\vec{E}^{-1}_{\text{prot}}| = 0.0028$, $|\vec{E}^{0}_{\text{prot}}| = 0.0038$, $|\vec{E}^{+1}_{\text{prot}}| = 0.0048$, $|\vec{E}^{+2}_{\text{prot}}| = 0.0058$, $|\vec{E}^{+3}_{\text{prot}}| = 0.0068$, $|\vec{E}_{\text{Fe-Fe}}| = |-\vec{E}_{\text{Fe-Fe}}| = 0.0038$.

Intermediate	no field	$\vec{E}^{-3}_{\text{prot}}$	$\vec{E}^{-2}_{\text{prot}}$	$\vec{E}^{-1}_{\text{prot}}$	$\vec{E}^{0}_{\text{prot}}$	$\vec{E}^{+1}_{\text{prot}}$	$\vec{E}^{+2}_{\text{prot}}$	$\vec{E}^{+3}_{\text{prot}}$	$\vec{E}_{\text{Fe-Fe}}$	$-\vec{E}_{\text{Fe-Fe}}$
[FeFe] − H$^-$ $\overset{\text{TS2}}{\rightarrow}$ [FeFe]$^{\mu}$ − H$^-$	−7.4	−7.5	−7.5	−7.5	−7.5	−7.6	−7.6	−7.6	−3.0	−10.1
[FeFe] − H$^-$ →TS2	29.6	29.4	29.4	29.4	29.4	29.4	29.4	29.3	33.2	27.0
[FeFe]$^{\mu}_{\text{Red}}$ → [FeFe]$^{\mu/\text{Lys}}_{\text{Red}}$ − H$^-$	11.3	11.5	11.6	11.8	12.0	12.2	12.4	12.6	5.5	17.6

4 Reaction energies with inverted field

Results for reaction energies obtained with inverted field directions are presented in Table 6.

Table 6: Reaction energies in kcal/mol for the different electric field strengths of the fields with inverted direction calculated with BP86-D3 (single point on structures optimized with BP86-D3 in vacuo). No continuum solvation model has been applied throughout. The field strengths in a.u. are: $|-\vec{E}^{-3}_{\mathrm{prot}}| = 0.0008$, $|-\vec{E}^{-2}_{\mathrm{prot}}| = 0.0018$, $|-\vec{E}^{-1}_{\mathrm{prot}}| = 0.0028$, $|-\vec{E}^{0}_{\mathrm{prot}}| = 0.0038$, $|-\vec{E}^{+1}_{\mathrm{prot}}| = 0.0048$, $|-\vec{E}^{+2}_{\mathrm{prot}}| = 0.0058$, $|-\vec{E}^{+3}_{\mathrm{prot}}| = 0.0068$.

Intermediate	no field	$-\vec{E}^{-3}_{\mathrm{prot}}$	$-\vec{E}^{-2}_{\mathrm{prot}}$	$-\vec{E}^{-1}_{\mathrm{prot}}$	$-\vec{E}^{0}_{\mathrm{prot}}$	$-\vec{E}^{+1}_{\mathrm{prot}}$	$-\vec{E}^{+2}_{\mathrm{prot}}$	$-\vec{E}^{+3}_{\mathrm{prot}}$
$[\mathrm{FeFe}]^{\mathrm{H}^+} \overset{\mathrm{TS1}}{\rightarrow} [\mathrm{H}] - \mathrm{H}^-$	−20.7	−21.9	−23.5	−25.1	−26.6	−28.1	−29.7	−31.2
$[\mathrm{FeFe}]^{\mathrm{H}^+} \rightarrow \mathrm{TS1}$	4.0	3.5	3.1	2.8	2.4	2.1	1.8	1.5
$[\mathrm{FeFe}]^{\mathrm{H}^+} - \mathrm{H}^- \rightarrow [\mathrm{FeFe}] - \mathrm{H}_2$	−6.4	−6.8	−7.4	−8.1	−8.7	−9.4	−10.0	−10.7
$[\mathrm{FeFe}] - \mathrm{H}^- \overset{\mathrm{TS2}}{\rightarrow} [\mathrm{FeFe}]^{\mu} - \mathrm{H}^-$	−7.4	−7.4	−7.4	−7.3	−7.3	−7.2	−7.1	−7.0
$[\mathrm{FeFe}] - \mathrm{H}^- \rightarrow \mathrm{TS2}$	29.6	29.4	29.3	29.3	29.3	29.3	29.2	29.2
$[\mathrm{FeFe}]^{\mu}_{\mathrm{Red}} \rightarrow [\mathrm{FeFe}]^{\mu/\mathrm{Lys}}_{\mathrm{Red}} - \mathrm{H}^-$	11.3	11.2	11.1	11.	10.9	10.8	10.7	10.7
$[\mathrm{FeFe}]_{\mathrm{Ox}} \rightarrow [\mathrm{FeFe}]_{\mathrm{Ox}} - \mathrm{O}_2$	−23.6	−24.4	−24.9	−25.5	−26.1	−26.6	−27.2	−27.7
$[\mathrm{FeFe}]_{\mathrm{Ox}} \rightarrow [\mathrm{FeFe}]_{\mathrm{Red}} - \mathrm{O}_2$	−17.2	−17.6	−18.1	−18.7	−19.2	−19.7	−20.2	−20.8
$[\mathrm{FeFe}]_{\mathrm{Ox}} \rightarrow [\mathrm{FeFe}]_{\mathrm{Red}}$	70.	93.8	124.5	155.1	185.7	216.3	246.8	277.4
$[\mathrm{FeFe}]^{\mu}_{\mathrm{Ox}} \rightarrow [\mathrm{FeFe}]^{\mu}_{\mathrm{Red}}$	71.1	95.5	126.5	157.6	188.7	219.8	251.	282.1

5 Discussion of partial charges

As a general trend it can be noted that both, $\mathrm{Fe_p}$ and $\mathrm{Fe_d}$, get more negatively charged with increasing $\vec{E}_{\mathrm{prot}}$ with exception of $[\mathrm{FeFe}]_{\mathrm{Ox}}$, $[\mathrm{FeFe}]^{\mu/\mathrm{Lys}}_{\mathrm{Ox}} - \mathrm{H}^-$ (where $\mathrm{Fe_d}$ gets more positively charged and $\mathrm{Fe_p}$ is unchanged) and $[\mathrm{FeFe}]^{\mu/\mathrm{Lys}}_{\mathrm{Red}} - \mathrm{H}^-$ (where both atoms get more positively charged). As a result of applying $\vec{E}_{\mathrm{Fe-Fe}}$ $\mathrm{Fe_d}$ gets more negatively charged for most intermediates and $\mathrm{Fe_p}$ more positively charged. Interestingly, $-\vec{E}_{\mathrm{Fe-Fe}}$ leads for most intermediates to a larger negative charge on both $\mathrm{Fe_p}$ and $\mathrm{Fe_d}$, although the whole $[2\mathrm{Fe}]_{\mathrm{H}}$ subcluster gets more positively charged. A table with partial charges on $\mathrm{Fe_p}$ and $\mathrm{Fe_d}$ for all intermediates and fields is given in Table 7.

From the subsequent Tables we understand: $\vec{E}_{\mathrm{Fe-Fe}}$ leads to a transfer of negative charge from the cubane to the $[2\mathrm{Fe}]_{\mathrm{H}}$ subcluster. $-\vec{E}_{\mathrm{Fe-Fe}}$ produces a transfer of negative charge from the the $[2\mathrm{Fe}]_{\mathrm{H}}$ subcluster to the cubane. If the

excess negative charge is on the $[2Fe]_H$ subcluster ($[FeFe]_{Red}$, $[FeFe]_{Red} - O_2$), $-\vec{E}_{Fe-Fe}$ leads to a larger shift of negative charge from the $[2Fe]_H$ subcluster to the cubane than $-\vec{E}_{Fe-Fe}$ in the opposite direction. If the excess negative charge is on the cubane (all other species), $\vec{E}_{Fe-Fe}$ leads to a larger shift of negative charge from the cubane to the $[2Fe]_H$ subcluster than $-\vec{E}_{Fe-Fe}$ in the opposite direction with the exception of $[FeFe]^{\mu}_{Ox}$ $[FeFe]^{\mu/Lys}_{Ox/Red}$. The field along the Fe–Fe bond is better suited to achieve a charge transfer between cubane and $[2Fe]_H$ subcluster because the magnitude of the charge shift is larger for $\vec{E}_{Fe-Fe}$ than for $\vec{E}^0_{prot}$ which have the same field strength.

Table 7: For each species the first row shows the partial charge on Fe_p and the second row the partial charge on Fe_d (measured in elementary charges e).

Intermediate		no field	$\vec{E}^{-3}_{\text{prot}}$	$\vec{E}^{-2}_{\text{prot}}$	$\vec{E}^{-1}_{\text{prot}}$	$\vec{E}^{0}_{\text{prot}}$	$\vec{E}^{+1}_{\text{prot}}$	$\vec{E}^{+2}_{\text{prot}}$	$\vec{E}^{+3}_{\text{prot}}$	$-\vec{E}_{\text{Fe-Fe}}$	$\vec{E}_{\text{Fe-Fe}}$
$[FeFe]_{Ox}$	Fe_p	−0.135	−0.138	−0.139	−0.140	−0.141	−0.143	−0.144	−0.145	−0.143	−0.134
	Fe_d	−0.124	−0.129	−0.127	−0.125	−0.123	−0.120	−0.118	−0.116	−0.112	−0.164
$[FeFe]_{Red}$	Fe_p	0.043	0.042	0.042	0.041	0.041	0.040	0.039	0.038	0.036	0.048
	Fe_d	0.027	0.027	0.026	0.026	0.026	0.025	0.024	0.024	0.029	0.024
$[FeFe]^{H^+}$	Fe_p	0.029	0.027	0.027	0.027	0.027	0.026	0.026	0.025	0.024	0.030
	Fe_d	−0.041	−0.044	−0.044	−0.045	−0.045	−0.046	−0.046	−0.046	−0.044	−0.045
$[FeFe] - H^-$	Fe_p	−0.141	−0.144	−0.145	−0.145	−0.146	−0.147	−0.148	−0.15	−0.151	−0.134
	Fe_d	−0.370	−0.379	−0.380	−0.381	−0.382	−0.383	−0.384	−0.385	−0.388	−0.367
$[FeFe]^{\mu} - H^-$	Fe_p	−0.160	−0.163	−0.163	−0.164	−0.164	−0.165	−0.165	−0.166	−0.170	−0.157
	Fe_d	−0.129	−0.155	−0.154	−0.153	−0.152	−0.151	−0.15	−0.149	−0.152	−0.160
$[FeFe]^{H^+} - H^-$	Fe_p	−0.145	−0.155	−0.156	−0.156	−0.156	−0.156	−0.156	−0.156	−0.165	−0.141
	Fe_d	−0.387	−0.403	−0.404	−0.405	−0.405	−0.406	−0.406	−0.407	−0.418	−0.381
$[FeFe] - H_2$	Fe_p	−0.119	−0.125	−0.125	−0.125	−0.126	−0.126	−0.127	−0.128	−0.140	−0.105
	Fe_d	0.401	−0.431	−0.432	−0.433	−0.434	−0.434	−0.435	−0.436	−0.450	−0.401
$[FeFe]_{Red} - H_2$	Fe_p	0.084	−0.091	−0.093	−0.094	−0.096	−0.097	−0.099	−0.101	−0.101	−0.082
	Fe_d	−0.327	−0.354	−0.358	−0.36	−0.363	−0.365	−0.368	−0.307	−0.367	−0.336
$[FeFe]_{Ox} - O_2$	Fe_p	−0.141	−0.142	−0.143	−0.144	−0.145	−0.146	−0.147	−0.149	−0.147	−0.135
	Fe_d	−0.169	−0.170	−0.170	−0.170	−0.170	−0.170	−0.171	−0.171	−0.175	−0.162
$[FeFe]_{Red} - O_2$	Fe_p	−0.087	−0.087	−0.088	−0.089	−0.089	−0.090	−0.091	−0.092	−0.097	−0.078
	Fe_d	−0.103	−0.103	−0.103	−0.103	−0.103	−0.103	−0.103	−0.103	−0.109	−0.102
$[FeFe]^{\mu}_{Ox}$	Fe_p	0.033	0.032	0.031	0.030	0.028	0.027	0.025	0.024	0.029	0.037
	Fe_d	0.089	0.089	0.088	0.088	0.088	0.088	0.088	0.087	0.087	0.089
$[FeFe]^{\mu/Lys}_{Ox} - H^-$	Fe_p	−0.210	−0.210	−0.210	−0.210	−0.210	−0.211	−0.211	−0.211	−0.211	−0.209
	Fe_d	−0.168	−0.167	−0.166	−0.165	−0.164	−0.163	−0.162	−0.161	−0.162	−0.175
$[FeFe]^{\mu/Lys}_{Red} - H^-$	Fe_p	−0.183	−0.183	−0.183	−0.182	−0.182	−0.182	−0.181	−0.181	−0.189	−0.178
	Fe_d	−0.172	−0.171	−0.170	−0.169	−0.168	−0.168	−0.167	−0.166	−0.169	−0.177

Table 8: For each species the first row shows the charge on the cubane and the second row the charge on the $[2Fe]_H$ subcluster (measured in elementary charges e). In columns two to nine the charge for no field and for the different field strengths are given.

Intermediate		no field	$\vec{E}^{-3}_{prot}$	$\vec{E}^{-2}_{prot}$	$\vec{E}^{-1}_{prot}$	$\vec{E}^{0}_{prot}$	$\vec{E}^{+1}_{prot}$	$\vec{E}^{+2}_{prot}$	$\vec{E}^{+3}_{prot}$	Δe_{max}	Δe^{inv}_{max}
$[FeFe]_{Ox}$	[4Fe4S]	−1.49	−1.47	−1.45	−1.42	−1.40	−1.37	−1.35	−1.32	+0.17	−0.10
	$[2Fe]_H$	−1.34	−1.35	−1.37	−1.39	−1.41	−1.43	−1.45	−1.47	−0.13	+0.06
$[FeFe]_{Red}$	[4Fe4S]	−1.66	−1.65	−1.63	−1.62	−1.60	−1.59	−1.57	−1.56	+0.10	−0.10
	$[2Fe]_H$	−1.94	−1.95	−1.96	−1.97	−1.97	−1.98	−1.99	−2.00	−0.06	+0.09
$[FeFe]^{H^+}$	[4Fe4S]	−1.50	−1.48	−1.46	−1.45	−1.44	−1.43	−1.41	−1.40	+0.10	−0.07
	$[2Fe]_H$	−1.31	−1.32	−1.33	−1.33	−1.34	−1.35	−1.35	−1.36	−0.05	+0.05
$[FeFe] - H^-$	[4Fe4S]	−1.51	−1.49	−1.48	−1.46	−1.45	−1.43	−1.41	−1.40	+0.11	−0.07
	$[2Fe]_H$	−1.32	−1.33	−1.34	−1.35	−1.35	−1.36	−1.37	−1.38	−0.06	+0.06
$[FeFe]^{\mu} - H^-$	[4Fe4S]	−1.52	−1.50	−1.49	−1.48	−1.46	−1.45	−1.43	−1.42	+0.10	−0.08
	$[2Fe]_H$	−1.32	−1.33	−1.34	−1.34	−1.35	−1.36	−1.37	−1.38	−0.06	+0.05
$[FeFe]^{H^+} - H^-$	[4Fe4S]	−1.35	−1.33	−1.31	−1.29	−1.27	−1.24	−1.22	−1.20	+0.15	−0.11
	$[2Fe]_H$	−0.66	−0.68	−0.69	−0.71	−0.72	−0.74	−0.76	−0.78	−0.12	+0.08
$[FeFe] - H_2$	[4Fe4S]	−1.15	−1.13	−1.11	−1.08	−1.06	−1.04	−1.02	−1.00	+0.15	−0.14
	$[2Fe]_H$	−0.90	−0.92	−0.94	−0.96	−0.97	−0.99	−1.01	−1.03	−0.13	+0.10
$[FeFe]_{Red} - H_2$	[4Fe4S]	−1.59	−1.57	−1.56	−1.54	−1.53	−1.51	−1.49	−1.48	+0.11	−0.08
	$[2Fe]_H$	−1.25	−1.26	−1.27	−1.28	−1.29	−1.29	−1.30	−1.32	−0.07	+0.05
$[FeFe]_{Ox} - O_2$	[4Fe4S]	−1.48	−1.47	−1.45	−1.43	−1.42	−1.40	−1.38	−1.37	+0.11	−0.09
	$[2Fe]_H$	−1.38	−1.39	−1.40	−1.41	−1.42	−1.43	−1.44	−1.45	−0.07	+0.07
$[FeFe]_{Red} - O_2$	[4Fe4S]	−1.76	−1.74	−1.73	−1.71	−1.70	−1.68	−1.66	−1.65	+0.11	−0.11
	$[2Fe]_H$	−1.89	−1.90	−1.91	−1.92	−1.93	−1.94	−1.95	−1.96	−0.07	+0.09
$[FeFe]^{\mu}_{Ox}$	[4Fe4S]	−1.35	−1.34	−1.32	−1.3	−1.28	−1.26	−1.24	−1.22	+0.13	−0.12
	$[2Fe]_H$	−1.49	−1.5	−1.51	−1.53	−1.54	−1.55	−1.57	−1.58	−0.09	+0.08
$[FeFe]^{\mu/Lys}_{Ox} - H^-$	[4Fe4S]	−1.14	−1.13	−1.11	−1.10	−1.08	−1.07	−1.05	−1.03	+0.11	−0.09
	$[2Fe]_H$	−1.20	−1.21	−1.22	−1.22	−1.23	−1.24	−1.25	−1.26	−0.06	+0.07
$[FeFe]^{\mu/Lys}_{Red} - H^-$	[4Fe4S]	−1.57	−1.56	−1.55	−1.53	−1.52	−1.51	−1.49	−1.48	+0.09	−0.09
	$[2Fe]_H$	−1.28	−1.29	−1.30	−1.30	−1.31	−1.32	−1.32	−1.33	−0.05	+0.05

Table 9: For each species the first row shows the charge on the cubane and the second row the charge on the $[2Fe]_H$ subcluster for the different field strengths of the fields with inverted direction (measured in elementary charges e).

Intermediate		no field	$-\vec{E}^{-3}_{prot}$	$-\vec{E}^{-2}_{prot}$	$-\vec{E}^{-1}_{prot}$	$-\vec{E}^{0}_{prot}$	$-\vec{E}^{+1}_{prot}$	$-\vec{E}^{+2}_{prot}$	$-\vec{E}^{+3}_{prot}$
$[FeFe]_{Ox}$	[4Fe4S]	−1.50	−1.50	−1.52	−1.54	−1.55	−1.57	−1.59	−1.60
	$[2Fe]_H$	−1.31	−1.33	−1.31	−1.30	−1.29	−1.27	−1.26	−1.25
$[FeFe]_{Red}$	[4Fe4S]	−1.66	−1.67	−1.68	−1.70	−1.71	−1.73	−1.74	−1.76
	$[2Fe]_H$	−1.94	−1.93	−1.92	−1.91	−1.89	−1.88	−1.87	−1.85
$[FeFe]^{H^+}$	[4Fe4S]	−1.50	−1.50	−1.51	−1.52	−1.53	−1.55	−1.56	−1.57
	$[2Fe]_H$	−1.31	−1.31	−1.30	−1.29	−1.29	−1.28	−1.27	−1.26
$[FeFe] - H^-$	[4Fe4S]	−1.52	−1.51	−1.53	−1.54	−1.55	−1.57	−1.58	−1.59
	$[2Fe]_H$	−1.32	−1.31	−1.30	−1.29	−1.28	−1.27	−1.27	−1.26
$[FeFe]^{\mu} - H^-$	[4Fe4S]	−1.52	−1.52	−1.54	−1.55	−1.56	−1.58	−1.59	−1.60
	$[2Fe]_H$	−1.32	−1.32	−1.31	−1.30	−1.30	−1.29	−1.28	−1.27
$[FeFe]^{H^+} - H^-$	[4Fe4S]	−1.35	−1.36	−1.37	−1.39	−1.41	−1.43	−1.44	−1.46
	$[2Fe]_H$	−0.66	−0.65	−0.64	−0.63	−0.61	−0.60	−0.59	−0.58
$[FeFe] - H_2$	[4Fe4S]	−1.15	−1.16	−1.18	−1.20	−1.22	−1.24	−1.26	−1.29
	$[2Fe]_H$	−0.90	−0.90	−0.88	−0.86	−0.84	−0.83	−0.81	−0.80
$[FeFe]_{Red} - H_2$	[4Fe4S]	−1.59	−1.59	−1.61	−1.62	−1.63	−1.65	−1.66	−1.67
	$[2Fe]_H$	−1.25	−1.25	−1.24	−1.23	−1.22	−1.21	−1.21	−1.20
$[FeFe]_{Ox} - O_2$	[4Fe4S]	−1.48	−1.49	−1.50	−1.52	−1.53	−1.55	−1.56	−1.57
	$[2Fe]_H$	−1.38	−1.37	−1.36	−1.35	−1.34	−1.33	−1.32	−1.31
$[FeFe]_{Red} - O_2$	[4Fe4S]	−1.76	−1.77	−1.79	−1.80	−1.82	−1.84	−1.85	−1.87
	$[2Fe]_H$	−1.89	−1.88	−1.87	−1.86	−1.84	−1.83	−1.81	−1.80
$[FeFe]^{\mu}_{Ox}$	[4Fe4S]	−1.35	−1.37	−1.39	−1.40	−1.42	−1.44	−1.45	−1.47
	$[2Fe]_H$	−1.49	−1.48	−1.47	−1.46	−1.44	−1.43	−1.42	−1.41
$[FeFe]^{\mu/Lys}_{Ox} - H^-$	[4Fe4S]	−1.14	−1.15	−1.17	−1.18	−1.20	−1.21	−1.23	−1.25
	$[2Fe]_H$	−1.20	−1.19	−1.18	−1.17	−1.16	−1.15	−1.14	−1.13
$[FeFe]^{\mu/Lys}_{Red} - H^-$	[4Fe4S]	−1.57	−1.58	−1.59	−1.61	−1.62	−1.63	−1.64	−1.66
	$[2Fe]_H$	−1.28	−1.28	−1.27	−1.26	−1.25	−1.25	−1.24	−1.23

Table 10: For each species the first row shows the charge on the cubane and the second row the charge on the $[2Fe]_H$ subcluster (measured in elementary charges e). In columns three and four show the charge for $\vec{E}_{Fe-Fe}$ and $-\vec{E}_{Fe-Fe}$, columns 5 and 6 the change in charge with respect to an absent field.

Intermediate		no field	$\vec{E}_{Fe-Fe}$	$-\vec{E}_{Fe-Fe}$	Δe_{max}	$\Delta e_{max,inv}$
$[FeFe]_{Ox}$	[4Fe4S]	−1.49	−1.30	−1.59	+0.19	−0.10
	$[2Fe]_H$	−1.34	−1.54	−1.22	−0.20	+0.12
$[FeFe]_{Red}$	[4Fe4S]	−1.66	−1.58	−1.74	+0.08	−0.16
	$[2Fe]_H$	−1.94	−2.00	−1.86	−0.06	+0.14
$[FeFe]^{H^+}$	[4Fe4S]	−1.50	−1.41	−1.56	+0.09	−0.06
	$[2Fe]_H$	−1.31	−1.39	−1.24	−0.08	+0.07
$[FeFe] - H^-$	[4Fe4S]	−1.51	−1.41	−1.57	+0.10	−0.06
	$[2Fe]_H$	−1.32	−1.41	−1.24	−0.09	+0.08
$[FeFe]^{\mu} - H^-$	[4Fe4S]	−1.52	−1.43	−1.58	+0.09	−0.06
	$[2Fe]_H$	−1.32	−1.42	−1.25	−0.10	+0.07
$[FeFe]^{H^+} - H^-$	[4Fe4S]	−1.35	−1.20	−1.45	+0.15	−0.10
	$[2Fe]_H$	−0.66	−0.82	−0.55	−0.16	+0.12
$[FeFe] - H_2$	[4Fe4S]	−1.15	−0.99	−1.29	+0.16	−0.14
	$[2Fe]_H$	−0.90	−1.08	−0.74	−0.18	+0.16
$[FeFe]_{Red} - H_2$	[4Fe4S]	−1.59	−1.49	−1.65	+0.10	−0.06
	$[2Fe]_H$	−1.25	−1.35	−1.17	−0.10	+0.08
$[FeFe]_{Ox} - O_2$	[4Fe4S]	−1.48	−1.35	−1.57	+0.13	−0.11
	$[2Fe]_H$	−1.38	−1.52	−1.27	−0.14	+0.11
$[FeFe]_{Red} - O_2$	[4Fe4S]	−1.76	−1.66	−1.89	+0.10	−0.13
	$[2Fe]_H$	−1.89	−1.99	−1.75	−0.10	+0.14
$[FeFe]^{\mu}_{Ox}$	[4Fe4S]	−1.35	−1.21	−1.48	+0.14	−0.13
	$[2Fe]_H$	−1.49	−1.65	−1.35	−0.16	+0.14
$[FeFe]^{\mu/Lys}_{Ox} - H^-$	[4Fe4S]	−1.14	−0.97	−1.33	+0.17	−0.19
	$[2Fe]_H$	−1.20	−1.26	−1.15	−0.06	+0.05
$[FeFe]^{\mu/Lys}_{Red} - H^-$	[4Fe4S]	−1.57	−1.50	−1.64	+0.07	−0.07
	$[2Fe]_H$	−1.28	−1.36	−1.22	−0.08	+0.06

6 Coordinates of the Structures

The coordinates are given in bohr.

Table 11: $[FeFe]^{H^+}$

39.86550906932277	39.96163812501639	29.63383492295196	h
50.18551979131814	38.72021940254938	52.89232550572605	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.81699518243870	37.26519818666974	31.43745744561616	h
37.17096426849932	21.01032619554276	48.96385247689395	h
32.35876564883519	20.70391307651310	50.61677155216560	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.28486351826432	44.92040742930136	49.78283639396901	h
47.92115865038991	26.90081067220600	42.61949169137408	h
46.86412249157463	42.98136402822649	46.43166503881454	c
47.44223897518989	40.91821485805941	44.82752561195316	o
36.34112639758646	30.49437944685234	40.23050456192303	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.11145777677385	27.90971236886144	42.73306786210922	c
41.49194610541505	26.98217852816664	42.12936362353613	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.27435129983814	19.70490683942119	41.54749572477420	s
42.40278700308750	32.25389949009116	45.58910689129356	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.00079378560793	27.95040661825460	48.14769715729721	fe
37.09977581314504	37.20117484513931	38.45385050716587	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.62676123397200	26.56355766398087	34.16288608621211	s
36.72961269650219	35.26018238126701	34.76214088587744	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
39.17201269464997	33.45321082953703	38.73771991547326	fe
34.12726761046917	34.01329098780811	38.83718210682007	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.08787322076494	20.86475825576595	51.40396146609547	o
42.88893434042153	37.83969570707317	42.57083039516254	h
40.55226970303312	21.97852870047579	56.13639975846672	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
43.88276515743119	25.44992646616500	44.74301503038872	h
47.53838911542930	39.43443030631705	49.56001680909265	h
50.66472411221336	43.43943705177877	47.92877500306450	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.76311741710400	24.69296682149825	57.13487807979616	h

36.28504762444758	30.32810995690647	36.07867761062767	fe
41.09416979998730	21.06590132172043	45.43615453392288	h
41.80508687496434	17.75507776932289	45.39755976256647	h
41.56317769812325	20.71864264631197	39.93573435561747	h
39.96840698439552	32.33175052998573	34.77696286244673	s
33.02131824731446	32.97206209489337	34.99281717250766	s
45.70792575636601	23.25600250058152	49.23478771594812	o
39.24692787735773	25.14333818876497	36.68803499811353	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.83488810638336	22.60257612449767	34.96048927993752	h
34.53563154641125	37.55325608825971	43.34488490654685	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.96114048266770	35.57096738672445	41.16331348623405	s
31.91274025718513	37.11074412163491	45.39557086286375	h
33.65068237628785	28.80809009038693	44.86833608092471	h
35.70865675509716	29.60408711010826	47.41696384408221	h
32.37108160374576	25.00158209577967	47.87172907810898	h
35.37105665783185	25.68262528629012	49.21722950621435	h
35.17294902503374	24.92293698205007	46.21054462728993	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.21588453664160	25.87157833837077	47.59937737147859	n
34.78789333218045	18.73839432312245	48.14917751000774	h
37.39195643088446	24.47069686105133	54.22992424024935	h
25.13256453229096	20.37153197990757	47.00797663948447	h
24.83705609893931	21.29297182254885	50.20978837348450	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.46721398149064	22.17962355209058	48.54932465033122	c
29.40742470031040	24.32584954682005	48.03094306403846	o
29.64518185589283	20.21087060161251	49.22504390038610	o
45.91680497813317	36.44980207849503	42.19453582351245	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.61538600540458	28.25126437092329	40.49091250059062	h
45.82951322239331	29.14384257844349	41.08367332414976	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.19357037765014	37.66300267246098	31.25936242497664	s
44.91519874382412	42.83642001344364	47.18196473493440	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.96422942634815	44.72108268560915	45.28522324425496	h
46.73880570260960	39.35417339236756	45.62580141753841	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.62570183798862	33.43853921088792	41.43718353676626	s
44.05521080351531	25.96641429047376	42.76864764207949	n
46.03538874984482	29.85051218568519	45.61345150865289	s
40.26389452945364	25.37176568685401	41.67211080270578	h

40.22033591891109	28.64933709124680	44.89356419845496	s
39.69136864922962	33.88850022883923	46.45693074579021	c
37.90680797685949	35.04307512172330	47.05777420351858	o
44.32166893332441	34.98356428466352	46.88487372859223	c
45.49385782162410	36.76456543041524	47.56153899933777	n
43.74722894487771	30.04830284303831	50.63988134322982	c
44.25806606952623	31.24397535214801	52.41964353732237	o
40.15396313719123	26.80063943719367	49.91303973205869	c
38.34277318748229	26.00327489410157	50.95053313613258	n
44.58130194277340	25.11446758466611	48.72879130022598	c
44.47684994924666	24.35882305712736	41.73834604162391	h

Table 12: $[FeFe]^{H^+} - H^-$

39.88027219052778	39.95638484457017	29.63462031514473	h
50.18591790742596	38.72099296038720	52.89659724568852	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.79886015194419	37.25401039524643	31.44824869364497	h
37.16932325472249	20.84065510452179	48.71957604094586	h
32.52159146393396	20.99665554953952	50.84618845043922	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.46300701504815	44.91771038205766	49.83287573225202	h
47.96127745462134	27.04953331921303	42.20815024092838	h
46.70021656135332	43.13069688650311	46.57561225109031	c
47.06600581208183	41.11002612020432	44.84376392193698	o
36.29152090884043	30.44226170841802	40.14531906752063	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.11774104288056	27.97240343487136	42.42246107562851	c
41.53089802028904	26.89472053058734	41.85395729727187	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.27873804344440	19.71221912412268	41.54593685381056	s
42.37221549670083	32.10034920598904	45.53724470053022	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.00313994338445	27.97778472599124	47.86587427696630	fe
37.16341841847144	36.88306343216814	38.49793216314217	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.38703766697773	26.31537368893769	34.12600605811428	s
36.52431283007441	35.09759351206613	34.52362148057197	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
34.12478783011036	34.06681169440390	39.00255249761528	fe
36.18544051593157	30.11962512744925	35.81958585288303	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.33428375495030	21.13508040500743	51.42089998648389	o
42.80332331097946	37.79149192400843	42.53391307886646	h
40.56049459822916	21.98825176438486	56.13898696797435	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.02801857282352	25.33403264323224	44.38231472430510	h
47.56867009200424	39.43434012536699	49.55724932456361	h
50.61325785478093	43.35198579260162	47.78405694192393	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.70109148295501	24.58607826839909	57.10680346179367	h
39.21351659606071	33.09346932638870	38.82710570394389	fe
41.08076935297919	21.06704986674231	45.43416656920771	h
41.79656545505078	17.75141340824964	45.39715860155135	h
41.51731169331262	20.45176304099078	39.84577299423113	h

39.75694603997304	32.09199533307262	34.63611983714317	s
33.00460015299183	32.96507139845028	34.95918009640052	s
46.48101434431327	27.16817911367397	52.05784093639915	o
39.16694654812960	25.31710799909564	36.64999939835042	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.96616435419872	22.60198999165990	35.02190360255885	h
34.52788393926121	37.55958926425264	43.28759718480084	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.90565529207788	35.48382179937969	41.28084105116928	s
31.97002863005782	37.14306068648829	45.41994982878668	h
33.71065685459562	28.93048351685893	44.87545082184230	h
35.73108422637328	29.49614334564203	47.53120331241702	h
32.10928729363503	24.99008466963175	47.63899223101158	h
35.11052059537702	25.46047059232177	49.08497644315852	h
35.01352847825954	24.89669333745949	46.04820253923394	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.06016896036906	25.82398475884837	47.45332285128870	n
34.57891687361903	18.68875699667020	48.33422458409427	h
37.27859961704729	24.25444758957508	54.19990798212408	h
25.24105195537209	20.42273540233027	46.92302501656936	h
24.78285922837365	21.20354867905846	50.15093583163834	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.44679603230346	22.28171665196397	48.64203103919753	c
29.36876388398004	24.30793598669001	47.70083925900863	o
29.64881687217525	20.55112213416455	49.75267930991216	o
45.90273791471996	36.51356428256886	42.22885888571659	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.58560173804027	28.19024268601153	40.22952658886248	h
45.74098149254182	29.26814092377309	40.83856622894535	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.20011585004301	37.71216917439460	31.25796595610304	s
44.80593019147150	43.03892478213246	47.46132965297539	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.79124464047878	44.89731714404968	45.47693347972255	h
46.47515237266622	39.52767921352780	45.65542964018069	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.72227510530318	33.40495939979093	41.31165404269372	s
44.13414712837736	25.95572334583989	42.44087360968657	n
46.10800013284381	29.75702016313552	45.37821859736875	s
40.35197029774125	25.25535186573843	41.38022238245529	h
40.18480145314942	28.46048313040566	44.60671571913852	s
39.55882047746860	33.85087323689648	45.80148145043939	c
37.73227937649820	35.03393717082353	45.99968976411265	o
44.28898659912767	34.89028268380505	46.75080857069632	c

45.43684258219919	36.65162130689886	47.47167900037656	n
41.93043643117277	31.23452502853679	49.23054107755314	c
41.32116573490397	32.25459024888885	51.09617486631017	o
40.27766662283800	26.52683616230891	49.64703285490692	c
38.51896775104967	25.63177141564384	50.66635303308325	n
45.10251123239360	27.55011147442076	50.39763854903288	c
43.60578711701084	25.16514823491901	47.29828305682668	h
44.57602845770754	24.40121403896081	41.33830496164635	h

Table 13: $[FeFe]_{Ox}$

39.96793997992780	39.93990211341126	29.65457256988891	h
50.18840278448362	38.71819795305516	52.88880440956434	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.75207994576776	37.19937971297082	31.46487350584901	h
37.16982250664979	20.91241983620206	48.81837968975515	h
32.44549963526131	20.85371171467688	50.80459712041704	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.25905666155342	44.91467605732352	49.77957187569801	h
47.90106694443463	26.81336556150879	42.58381037598530	h
46.89894329062441	42.98506726246194	46.40450967810271	c
47.54080766623974	40.96506152868516	44.76714891819752	o
36.32044919497505	30.52579489502083	40.18700837069380	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.03586190563896	27.72281515642321	42.64765666284433	c
41.57624431093509	26.83504260988860	42.04738704896624	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.56365793823410	19.19628017359813	41.80456858026132	s
42.42639807949946	32.24524535779574	45.60520843956193	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.86301930067923	28.25674215523115	48.22715808456353	fe
37.06099506883753	37.14684343696987	38.45172200299144	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.56787332460085	26.48610657063465	34.12849350163285	s
39.27987558000863	33.42784541544735	38.72427342254701	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
33.96852440569990	34.02748952997807	38.88712813027284	fe
36.17081501121968	30.23202940998607	36.02421194816880	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.23624001610162	21.01990745819170	51.43408378991365	o
42.80405228667493	37.78485277129020	42.54081910664169	h
40.55638179798955	21.98689354443379	56.13659355264133	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.09569899036929	24.75772526219302	44.04252398693810	h
47.56231085981603	39.42966850075850	49.54241313673744	h
50.67086687172961	43.45543710250796	47.95352574166446	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.72548782178207	24.63216807899619	57.11601970596425	h
36.65055033394117	35.37512692902988	34.64485171665672	fe
41.11649851116378	21.21185827906404	45.18289244514835	h
41.58758077795893	17.93608796125428	45.71211024645281	h
43.70669130863487	21.71748284969796	41.27554353102161	h

39.82832323436102	32.33489396516544	34.70975625014576	s
32.95394556699983	33.00215059072229	34.99238368939979	s
46.41637715816767	27.64856403751996	52.39964691238362	o
39.21666046167534	25.19640061567065	36.68337487673232	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.88038976526538	22.60155342275371	34.98396873896520	h
34.52254675212102	37.53895215927541	43.24279944974531	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.83762616181052	35.55467358761777	41.26506688938464	s
32.00299002747607	37.13883666737827	45.42717167214791	h
33.67325847812189	28.86472374142534	44.87001049063317	h
35.72010210232583	29.56581969270245	47.44924665603154	h
32.32262775288810	24.96813492785430	47.72362355102386	h
35.28512116342255	25.55868945972380	49.13671350414094	h
35.17028439653282	24.94764273775487	46.10528477429285	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.18615660461091	25.84619239238032	47.51043031878046	n
34.65913615643555	18.70912389638379	48.25510902367831	h
37.33876213249809	24.34940457946115	54.20459992341000	h
25.22245238002981	20.42036349914560	46.92689611946531	h
24.76366278167775	21.21102490984292	50.14739950702351	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.45293352152798	22.21759130977301	48.66046283639394	c
29.42265971065132	24.25436836290910	47.83109038602612	o
29.58928253227038	20.38962332427034	49.69371027948281	o
45.90591866810603	36.52984029825496	42.22068438325879	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.56453934731688	28.14951909489901	40.43649946234608	h
45.85931235268531	29.06909384239114	41.07202380681206	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.15631703238873	37.82576534189631	31.18946293066633	s
44.94218857997730	42.78894959548398	47.12208593091590	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.98179833257475	44.74593863217058	45.29093375689262	h
46.88233448771184	39.37660121171643	45.54242795823738	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.77474452420240	33.37353657634117	41.35515391321535	s
44.08867676808882	25.80948257267620	42.40879717037127	n
46.06420401806162	29.62589030676375	45.62178889658261	s
40.24148350569899	25.30113301697005	41.62652047449055	h
40.19139631475603	28.50914720456817	44.80389842215027	s
39.65554935420511	34.04161712248852	45.79180566632217	c
37.84301287223913	35.26870511257474	45.93118619612332	o
44.42948131582691	34.99370838741342	46.74022519338619	c

45.62254100758037	36.74760666772085	47.42703481515836	n
41.86554815258874	31.50548938945350	49.30732931706211	c
41.20244892450686	32.61756108866811	51.12382855471220	o
40.20145154746713	26.62753934300755	49.92545873254752	c
38.45119665912869	25.62835232359556	50.87914114686966	n
44.99271607710737	27.90057980327523	50.73274784341865	c

Table 14: $[FeFe]_{Red}$

40.01285230301865	39.93046543739169	29.65190131998337	h
50.18834269096357	38.71711587048926	52.88377128127341	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.74148288537657	37.17562076438909	31.46300018009511	h
37.14362413770955	21.12048715949495	49.14717878802350	h
32.25938919178008	20.49570354249268	50.46593137012365	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.16222627199618	44.91241438118081	49.74478642222371	h
47.89356679149522	26.40226431363806	43.26602101526484	h
46.99255655292402	42.89429481817044	46.33572614334226	c
47.73899034256621	40.84827135614059	44.79405018071927	o
36.34042412463823	30.45947029755304	40.16799921121920	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.08176045562364	27.41332308711388	43.13303187786980	c
41.59099612773223	26.71267273983491	42.49913192491015	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.45871444680086	19.57383109363088	41.69707813376673	s
42.52545133701980	32.29377166187670	45.64690467523670	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.91077449893299	28.28104537347795	48.55782006939391	fe
37.07317081122616	37.12318727023626	38.50110620694391	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.58294876703322	26.46057879526319	34.08316955918066	s
39.29039021996000	33.38484547265385	38.79003861316978	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
33.99091978416194	33.98018856400846	38.89963382901533	fe
36.23318752984823	30.23081166731801	35.99571400302604	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
33.92340026327805	20.65196317503997	51.37733515707584	o
42.81765425727082	37.79103984973872	42.55116862080862	h
40.54510281332288	21.96792125969776	56.13489518885972	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
43.89770364620605	24.86215673397928	44.88099636967797	h
47.55415168659661	39.41802959475759	49.53107839528122	h
50.69088442766103	43.50543284018070	48.03144975234412	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.82588623665130	24.76992756425711	57.17271074419961	h
36.68541735911251	35.37044248590485	34.68960624989793	fe
41.06255398847827	21.13246552551844	45.32762288771142	h
41.67529381041695	17.84362670782804	45.58359689748914	h
43.93522078673323	22.17377777102560	41.89843533904217	h

39.90625826131605	32.36636921712573	34.71590460359350	s
32.98362763827347	32.99135756724340	34.97296472051485	s
45.69986733748413	23.81194817329549	50.21797835238517	o
39.20157826694213	25.21195834686752	36.70380740090661	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.91522044857538	22.59269227542973	35.00859072322817	h
34.52495557785005	37.53258754105656	43.24821373977228	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.83341773190607	35.56878159373109	41.25145863302730	s
32.00175527165806	37.13790303811783	45.42742540210523	h
33.58542853213483	28.67499988023146	44.86927893917529	h
35.68144711670721	29.70306126594221	47.28630448689910	h
32.62729251908315	24.97424174192024	47.99590307615637	h
35.52571507948829	25.92570706063525	49.39547189751859	h
35.45609410208959	25.01014298294743	46.41157557938472	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.38329883658837	25.93618291538256	47.73282392662412	n
34.94517527536551	18.79693184132139	48.03113561081946	h
37.46700177078762	24.64750912796449	54.26947219993674	h
25.05660698251462	20.34955524008199	47.05795984495787	h
24.87569810514776	21.34898395443634	50.24381271730093	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.48172360628400	22.09988917320483	48.48151894822119	c
29.46761217813293	24.24838534181553	48.14016416874028	o
29.59848500794083	20.03493750228703	48.96290677013736	o
45.90672947663386	36.52977393702675	42.22259417405891	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.72951735093948	27.91003946709564	40.80531271174846	h
46.03564181056896	28.54884077365540	41.39059966465074	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.16263697073610	37.87937197225247	31.20691864809582	s
45.01494595674696	42.67241299483423	46.98799904388431	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.07964404797089	44.63784347447564	45.18832116126417	h
47.00952969233722	39.26359844741706	45.56832865674530	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.77452229515585	33.36519600862098	41.44091191049100	s
44.03651887209238	25.56598097260940	43.05802673524830	n
46.04366880857530	29.69533496184690	45.83523564710595	s
40.20215272586292	25.21387099401035	42.11825403383932	h
40.27404946396730	28.64615557167147	45.10995518996373	s
39.84172927538263	33.98905696246188	46.46344732211236	c
38.05979543662863	35.17473217416425	47.04038649544452	o
44.51323006733167	35.01610642859612	46.83970162699729	c

45.70952819058878	36.80748066735516	47.47415790991580	n
43.63146569496969	30.59759003407171	50.83337453264873	c
44.10489175487744	31.93817220087622	52.53195338162597	o
40.02030379685256	27.25341008113662	50.29310831430343	c
38.17908688589988	26.46218497763958	51.30306752751279	n
44.51351557783531	25.54968538631328	49.47284539976413	c

Table 15: $[FeFe]^{\mu} - H^{-}$

39.96576679488405	39.94031029425426	29.65346519037966	h
50.18467057538677	38.71987414012803	52.89331329609858	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.75065698199565	37.19874098554057	31.46531003258389	h
37.16704649897218	20.82791128389235	48.70608271477741	h
32.51398142030496	20.98038383628746	50.90413088514657	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.36251160799232	44.92214236524337	49.80221457412768	h
48.20052239483174	27.13766902072344	42.47964489252340	h
46.77967889542382	43.02361389595956	46.49820607883215	c
47.25411731581696	40.94875886140484	44.87583273682427	o
36.36196269848890	30.49076126238957	40.21549221257583	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.29136988527323	27.95016621679506	42.51314973671954	c
41.88393518778492	26.78345686612852	41.89191928066302	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.58345659884566	19.09691081504147	41.85212542792291	s
42.37968404968962	32.12504176871102	45.50135287118452	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.12050771329248	28.02216100270507	48.15667507955352	fe
37.02845209523902	37.13972105920476	38.44948267753332	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.55839823781012	26.46822598203996	34.11832299562814	s
36.61283706966468	35.35107827436320	34.64965917991871	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.18484244824550	30.20782201832490	36.03644225564976	fe
33.96749072550953	33.98439621542372	38.90726127240852	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.34308891066100	21.13949121710742	51.42646630390380	o
42.80230051055706	37.78518725281432	42.53908055860671	h
40.55153842993119	21.97496559313283	56.13619859988120	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.66584636981499	24.57740192616775	43.38872599084345	h
47.53671829890525	39.43913035946634	49.56268233915412	h
50.64090337429172	43.39517562610804	47.85803410111628	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.75972398998857	24.68630306329888	57.13398533223457	h
39.27813136279526	33.43605060628208	38.71891982843491	fe
41.15250346302328	21.22001811647177	45.15972251312981	h
41.58985411848730	17.95190685864660	45.72614335265701	h
43.06648611255729	21.26978216424735	40.60347188329827	h

39.82402032797441	32.33481270694206	34.69498426102668	s
32.94300216301000	32.95030028530472	35.01222014453386	s
45.90375871114516	29.25787370282575	52.77444574338423	o
39.21005586886849	25.21112725136273	36.68309330753969	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.89500868656832	22.59907221235159	34.99138591400580	h
34.52386578095626	37.53335856994543	43.24407312515356	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.83586304733590	35.54858489004304	41.27126519107463	s
32.00414276041231	37.14059411267451	45.42788787834927	h
33.64120116413751	28.79453175423857	44.86674126443693	h
35.71358632664685	29.60358775903658	47.40001173157096	h
32.37878474414454	24.96341439199407	47.75847765967324	h
35.25075649383955	25.69393526876347	49.27853556009559	h
35.29538426600740	24.95885826230671	46.26549197571756	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.22446702234290	25.87214400125486	47.59627868691279	n
34.57705590219646	18.68929500015423	48.33404855309767	h
37.36761069152224	24.46939085004150	54.23452751605153	h
25.29305443778570	20.45477352215561	46.87670310385936	h
24.71696386967691	21.15983789829522	50.10408698423866	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44852290075224	22.25732658100325	48.74801384776489	c
29.44676316737561	24.21022625035538	47.76819652113409	o
29.55737639637599	20.53707298462521	49.98271743413483	o
45.90333730221928	36.52777293787421	42.22908421588437	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.65523486295982	28.16523405735446	40.35379937793799	h
46.10679655519284	29.39387162286317	41.02556111057683	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.15700867215048	37.82395498426857	31.19246759520507	s
44.85629296869184	42.92447508399014	47.31833587872261	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.87882337657160	44.75943883560754	45.34645013099267	h
46.53126494766278	39.39731261004636	45.67398124242882	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.77009201848266	33.37863883687865	41.33833157125065	s
44.47534685860663	25.97482793943476	42.06709311299768	n
46.11669683036169	29.80324488304665	45.53738238948365	s
40.66734651604918	25.15118891813018	41.47948277443092	h
40.44560227309017	28.32251218328543	44.73230803763101	s
39.51682077991708	33.66261743031206	46.00391419576982	c
37.61421617138165	34.70013187499116	46.39266298502513	o
44.18753212113948	34.93695046324924	46.81311948893170	c

45.30395774934607	36.72368651443067	47.55625617731155	n
42.18202625591979	31.16495507255128	48.44777794047815	h
44.86113444702407	22.79752180136779	48.08344819221002	o
40.17556040982859	27.13143670396322	50.01925906821383	c
38.34496381528606	26.43893522710256	51.07622635362362	n
44.82281269093533	28.79010223620159	50.92429048344800	c
44.13487112321428	24.88193696038885	48.05326170708937	c

Table 16: $[FeFe]^{H^+} - H^-$

39.88027219052778	39.95638484457017	29.63462031514473	h
50.18591790742596	38.72099296038720	52.89659724568852	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.79886015194419	37.25401039524643	31.44824869364497	h
37.16932325472249	20.84065510452179	48.71957604094586	h
32.52159146393396	20.99665554953952	50.84618845043922	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.46300701504815	44.91771038205766	49.83287573225202	h
47.96127745462134	27.04953331921303	42.20815024092838	h
46.70021656135332	43.13069688650311	46.57561225109031	c
47.06600581208183	41.11002612020432	44.84376392193698	o
36.29152090884043	30.44226170841802	40.14531906752063	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.11774104288056	27.97240343487136	42.42246107562851	c
41.53089802028904	26.89472053058734	41.85395729727187	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.27873804344440	19.71221912412268	41.54593685381056	s
42.37221549670083	32.10034920598904	45.53724470053022	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.00313994338445	27.97778472599124	47.86587427696630	fe
37.16341841847144	36.88306343216814	38.49793216314217	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.38703766697773	26.31537368893769	34.12600605811428	s
36.52431283007441	35.09759351206613	34.52362148057197	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
34.12478783011036	34.06681169440390	39.00255249761528	fe
36.18544051593157	30.11962512744925	35.81958585288303	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.33428375495030	21.13508040500743	51.42089998648389	o
42.80332331097946	37.79149192400843	42.53391307886646	h
40.56049459822916	21.98825176438486	56.13898696797435	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.02801857282352	25.33403264323224	44.38231472430510	h
47.56867009200424	39.43434012536699	49.55724932456361	h
50.61325785478093	43.35198579260162	47.78405694192393	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.70109148295501	24.58607826839909	57.10680346179367	h
39.21351659606071	33.09346932638870	38.82710570394389	fe
41.08076935297919	21.06704986674231	45.43416656920771	h
41.79656545505078	17.75141340824964	45.39715860155135	h
41.51731169331262	20.45176304099078	39.84577299423113	h

39.75694603997304	32.09199533307262	34.63611983714317	s
33.00460015299183	32.96507139845028	34.95918009640052	s
46.48101434431327	27.16817911367397	52.05784093639915	o
39.16694654812960	25.31710799909564	36.64999939835042	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.96616435419872	22.60198999165990	35.02190360255885	h
34.52788393926121	37.55958926425264	43.28759718480084	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.90565529207788	35.48382179937969	41.28084105116928	s
31.97002863005782	37.14306068648829	45.41994982878668	h
33.71065685459562	28.93048351685893	44.87545082184230	h
35.73108422637328	29.49614334564203	47.53120331241702	h
32.10928729363503	24.99008466963175	47.63899223101158	h
35.11052059537702	25.46047059232177	49.08497644315852	h
35.01352847825954	24.89669333745949	46.04820253923394	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.06016896036906	25.82398475884837	47.45332285128870	n
34.57891687361903	18.68875699667020	48.33422458409427	h
37.27859961704729	24.25444758957508	54.19990798212408	h
25.24105195537209	20.42273540233027	46.92302501656936	h
24.78285922837365	21.20354867905846	50.15093583163834	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.44679603230346	22.28171665196397	48.64203103919753	c
29.36876388398004	24.30793598669001	47.70083925900863	o
29.64881687217525	20.55112213416455	49.75267930991216	o
45.90273791471996	36.51356428256886	42.22885888571659	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.58560173804027	28.19024268601153	40.22952658886248	h
45.74098149254182	29.26814092377309	40.83856622894535	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.20011585004301	37.71216917439460	31.25796595610304	s
44.80593019147150	43.03892478213246	47.46132965297539	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.79124464047878	44.89731714404968	45.47693347972255	h
46.47515237266622	39.52767921352780	45.65542964018069	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.72227510530318	33.40495939979093	41.31165404269372	s
44.13414712837736	25.95572334583989	42.44087360968657	n
46.10800013284381	29.75702016313552	45.37821859736875	s
40.35197029774125	25.25535186573843	41.38022238245529	h
40.18480145314942	28.46048313040566	44.60671571913852	s
39.55882047746860	33.85087323689648	45.80148145043939	c
37.73227937649820	35.03393717082353	45.99968976411265	o
44.28898659912767	34.89028268380505	46.75080857069632	c

45.43684258219919	36.65162130689886	47.47167900037656	n
41.93043643117277	31.23452502853679	49.23054107755314	c
41.32116573490397	32.25459024888885	51.09617486631017	o
40.27766662283800	26.52683616230891	49.64703285490692	c
38.51896775104967	25.63177141564384	50.66635303308325	n
45.10251123239360	27.55011147442076	50.39763854903288	c
43.60578711701084	25.16514823491901	47.29828305682668	h
44.57602845770754	24.40121403896081	41.33830496164635	h

Table 17: [FeFe] – H_2

39.85842657153217	39.96068532133395	29.64630312836593	h
50.18531119254314	38.72027287234040	52.89499515234981	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.79104987791738	37.26066920038274	31.45607494101105	h
37.16278705628644	20.81300134476615	48.68085487100874	h
32.54642423841885	21.04046767843163	50.87795817831542	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.44515311089054	44.91713081155988	49.82778634805110	h
48.23117564230527	27.29455786307266	42.12533447216997	h
46.71016154046368	43.11308675879962	46.56316163492654	c
47.08695970170452	41.08060127369340	44.84887579365124	o
36.43242113705929	30.58632849198274	40.25433553307508	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.33239772917296	28.12356937575060	42.21450308910393	c
41.91141558509458	27.02270186273108	41.45946679531499	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.46592319277556	19.67905039647637	41.74914102328913	s
42.38797616792609	31.96124030819658	45.57496904210978	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.12351048810509	27.68253564406897	47.80991789452170	fe
37.05926785915929	37.16790632435904	38.46599699413964	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.61644873464380	26.57243303947661	34.18806900744940	s
34.01176700861813	34.05320492308699	38.95154322469550	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.26170894810575	30.23941256995642	36.12177094909772	fe
36.63147732816162	35.38645772687534	34.67134000775076	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.36944114147404	21.17036745226369	51.42031713509307	o
42.80426582572705	37.78245659856371	42.54215325328594	h
40.55983621734604	21.98630394988279	56.13872327398419	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.42758214107129	25.08873724915140	46.61672781166562	h
47.57124170548276	39.43385991330373	49.55536154014590	h
50.61666763673868	43.35837887900217	47.79468481222813	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.70514303032039	24.59215501802558	57.10951337891590	h
39.35433456878563	33.54207746997709	38.73332710041186	fe
41.03180854514606	21.05785882795994	45.44414897165484	h
41.73514949105968	17.76094814398988	45.44952335275433	h
42.13980977428743	21.30073965762699	40.28310850305423	h

39.80843008744321	32.38900816248076	34.72570931809295	s
33.03525670270606	32.92248162701870	35.08343825300649	s
46.32135416969849	27.57190540753347	52.31828286434590	o
39.25650344729471	25.12848007928613	36.65959456317540	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.79905973229790	22.61686020436616	34.93408752816987	h
34.52688745303013	37.53689802697755	43.27999870851581	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.85860401152407	35.59090530661227	41.21619290261393	s
31.95757612924022	37.11474265928460	45.40641492039097	h
33.70121508641505	28.92503435070451	44.87500881623378	h
35.73993099855539	29.49097519979596	47.51150746267171	h
32.12522885159741	24.97982855311577	47.59551901701055	h
35.08729329430147	25.47105719012947	49.09467087731208	h
35.06133412652244	24.91426639493524	46.05440767782965	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.06580939634069	25.82405047137378	47.44289717625156	n
34.55195467007817	18.68284536488962	48.36093179695182	h
37.27540150525318	24.27100362198742	54.20180312874501	h
25.25753703526645	20.43255601210407	46.90750752942288	h
24.77141065879022	21.18931195666675	50.13929825112567	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44406503682339	22.29537243707775	48.65727297869495	c
29.37172781213049	24.28029918479626	47.63765990959790	o
29.63689229226347	20.61466135986520	49.85127942323702	o
45.90607173592215	36.52757262690496	42.21949385580003	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.65693372674620	28.54741226887316	40.06880600157545	h
46.19450819328442	29.71883081704319	40.88786432675305	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.16530268011307	37.68992615885340	31.19562532755993	s
44.81118331636212	43.02579086045554	47.43964495759045	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.80485382686098	44.87246146541729	45.45296643375406	h
46.47898945386708	39.50226799902850	45.66011065267136	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.77677975923901	33.38571775094287	41.29435386486980	s
44.49879647009168	26.24641748839272	41.56108114850814	n
46.17186549485475	29.65942160712564	45.42493045696366	s
40.71869604404363	25.42495165213188	40.88448549644156	h
40.38264604723601	28.21227123033167	44.44217649593462	s
39.48501668923343	33.58716633531944	45.71966537150054	c
37.59114639484773	34.67023640769377	45.85596186826570	o
44.26608614642934	34.82476687183900	46.70716821428169	c

45.38148943280230	36.61932827890403	47.39439357580135	n
42.01490643632985	31.25345094698473	49.03116474115555	c
41.45436075532525	32.06024683933725	51.01850466913569	o
40.25836064972131	26.52086808270391	49.63948836777836	c
38.44792365348020	25.80007740575211	50.70371976041263	n
45.07075042771287	27.62285620331555	50.52062419616200	c
43.12760363489183	24.59818513409044	47.40768590936456	h
44.72395355843241	24.60192490209180	42.55105386333466	h

Table 18: $[FeFe]_{Red} - H_2$

39.98087704497950	39.93713366463815	29.65754510908352	h
50.18768657828225	38.71881211404578	52.89043335348408	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.73887076015406	37.18930558299847	31.47128156713887	h
37.17025525393241	20.93704107788460	48.84998157974342	h
32.42496587118713	20.82323988091136	50.74617434753674	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.27359243490687	44.91615760260551	49.78191702581913	h
48.13212753718985	27.26872908639625	42.28934758201042	h
46.87768198199211	42.98059050127183	46.42024920699778	c
47.48211655224968	40.93030757552041	44.80753803466700	o
36.30545043872097	30.53105967200506	40.19525513550328	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.23057928555830	28.09155363574096	42.41961963188911	c
41.80014662112883	26.99751181348492	41.72191006982797	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.54450556395729	19.38677023617586	41.80366529117357	s
42.37566838167400	32.08164231852442	45.70505967828046	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.06297689114317	27.70837764882826	48.07575889660742	fe
37.00896145998583	37.15525082849997	38.42000861916180	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.55020438533216	26.46638916824647	34.12219882391050	s
36.59934064567997	35.36292307771467	34.62368678405680	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.14890930597875	30.22402264039448	36.02557444070491	fe
33.93804123357762	34.01761004179661	38.87865081887612	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.19932988542824	20.98185215348657	51.42618662443730	o
42.83077112435621	37.80394089487876	42.54995215300379	h
40.55410089855668	21.98194813116468	56.13579608821658	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.42154635582806	24.96900798132405	46.90807066780813	h
47.55275073534969	39.43572696271522	49.55165200776253	h
50.66664900301863	43.44380772793475	47.93896540187138	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.74439831111487	24.66207110519809	57.12636784622472	h
39.25512016777122	33.44706204041241	38.69501101350149	fe
41.08208848815377	21.14852032853263	45.30302044518807	h
41.65717372196406	17.84680407102671	45.59247168547947	h
42.63784331507724	21.37160816676650	40.46797663041010	h

39.79993198905912	32.32603492909146	34.68062045275061	s
32.91541027185897	32.97610071608926	34.98349819716008	s
46.24813484125949	27.63395267512151	52.57984363675852	o
39.20961178322912	25.21575330091671	36.67832174907408	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.89487262628733	22.60015880487346	34.98969838857619	h
34.52051340681052	37.53625740982117	43.22393431383950	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.82127247192482	35.54760790163642	41.28346715266371	s
32.01953835915263	37.14368192516275	45.43239865460964	h
33.67155016570491	28.86485980170633	44.86973648034505	h
35.72272315246120	29.56387327479371	47.44699977166893	h
32.32447023585998	24.97447684872978	47.72481974766098	h
35.28194831325870	25.58111861910135	49.14669503753316	h
35.17852549216391	24.95282436678961	46.11222951780221	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.18542717032666	25.84865659524732	47.51296444151408	n
34.69047159504019	18.71436032747614	48.22841097298440	h
37.35347742983341	24.40063883416198	54.21357990195597	h
25.18812739469543	20.40136797213717	46.95606215247847	h
24.79388517159477	21.23982055653558	50.17174673841794	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.45878411361096	22.20735844280617	48.61244300583172	c
29.41027633535423	24.28073193207889	47.86142993896289	o
29.61758496044440	20.33652390988414	49.54233754769244	o
45.91030094298989	36.49763936508506	42.20893784566582	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.57829277405458	28.47923095028339	40.28104492212574	h
46.03666314951596	29.65268473349004	41.06019601099572	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.14871466418788	37.84067717074863	31.17038425570839	s
44.92464814208510	42.81889041620838	47.15557187785079	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.97361959790578	44.72620800169953	45.28381137912751	h
46.76761677356798	39.36255109797710	45.57449850030466	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.72542456206619	33.39919338794021	41.31693609206347	s
44.39108586041929	26.17809255061745	41.83428074412458	n
46.13595502930150	29.66069717226001	45.61082470560541	s
40.58565743511794	25.40194423656008	41.17980433635106	h
40.31605776776961	28.28166764281981	44.67293095305759	s
39.51160324608597	33.74540633184802	45.82441667006118	c
37.62626317542849	34.85415400280877	45.96165047098434	o
44.29937745157336	34.92382631531115	46.77566889658657	c

45.46330512538390	36.71052646169622	47.42357661634964	n
41.98882632607882	31.30915440397117	49.14890034792103	c
41.40884670160478	32.14288267305709	51.13445070526080	o
40.20365118867662	26.53629391706223	49.86991779200783	c
38.37880125128019	25.78165446575954	50.90112244115559	n
44.99602876700449	27.66524465002528	50.76769643837429	c
43.09421784344156	24.50574162178187	47.57432762824487	h
44.58781957811399	24.65012047718363	43.00054411942563	h

Table 19: $[FeFe]_{Ox} - O_2$

39.95976138210226	39.94152064781136	29.65291540486628	h
50.19022852198461	38.71767233641628	52.88772349655026	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.75484710004186	37.20387681960462	31.46416472365701	h
37.17182003888116	20.84898861810825	48.74094667503127	h
32.50069715505579	20.94769065027657	50.88111515151999	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.23689648454624	44.91246171026754	49.77287248551643	h
47.98284615605807	26.91534212354711	42.41305274843909	h
46.91657816320334	42.96488474477126	46.39178573999541	c
47.57592096449700	40.93315495181069	44.77395496450163	o
36.34408599141050	30.56714957158233	40.22978689590221	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.10899397370236	27.80599062204659	42.46079784512339	c
41.66455409133112	26.86336069307466	41.84799295474632	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.55179399223472	19.01941975765925	41.81285812639342	s
42.43303832912363	32.11818240493694	45.61924794652298	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.95243880614457	27.95216875584354	48.07564642854300	fe
37.07091951228544	37.18069379893004	38.45883896710725	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.57530479370173	26.51414138558464	34.15216325851961	s
39.29951990171115	33.46522900778930	38.72882808458982	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.19563617442900	30.24266039750882	36.06373513368248	fe
33.97559973212935	34.04912921128597	38.89443709286562	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.31521147087607	21.11008539318031	51.43310120212084	o
42.78427454032399	37.77576112101227	42.53014236083857	h
40.55291445135855	21.98117061096567	56.13635012450320	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.26592659047557	24.66659335179115	43.61220134863073	h
47.57339094744228	39.42765565098756	49.54155455801156	h
50.67492341622506	43.46570066136764	47.97020851213851	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.75097162764080	24.67124458347579	57.13077738319361	h
36.64989630191939	35.38888516517000	34.65465845231116	fe
41.20813346643529	21.23668445424758	45.12384796583502	h
41.57856001393036	17.97957291432058	45.75515490508046	h
43.50781422868667	21.42962788886438	40.93817416911419	h

39.83681839503340	32.35091511615983	34.72086869463914	s
32.97569071781803	32.99743899155613	35.00762393232985	s
46.24260390112732	28.06648090185988	52.51932910713231	o
39.22880460721547	25.17529888575400	36.67719980304955	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.85633383267050	22.60544019240703	34.96909827646945	h
34.52184593498657	37.53896672492724	43.23738706674185	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.83026002451605	35.56477762137095	41.25862548613291	s
32.00232537461393	37.13458383795383	45.42546990168690	h
33.66214750363350	28.83176902604099	44.86780885080663	h
35.71971107480287	29.57382596222890	47.43665995582196	h
32.32342652286018	24.97596984522447	47.74304212592872	h
35.23309214814302	25.64559946819296	49.23512906079253	h
35.22543750952578	24.93621782435500	46.21604472787885	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.18545160209793	25.86094266618630	47.56292461646362	n
34.59544671192539	18.69727017272023	48.31340094183309	h
37.35325334798412	24.43499629940070	54.22475340667540	h
25.27541549004626	20.44428354292789	46.89053884791193	h
24.72994059035879	21.17267428566641	50.11593232978974	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44556917182217	22.25340509415384	48.72261969505865	c
29.41983320077650	24.24999785488354	47.80264794470553	o
29.57152879486874	20.49438440634039	49.87786535162657	o
45.90425230109432	36.55286724839543	42.22393468122988	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.55517363427791	28.23873810944571	40.29144588009638	h
45.96683471228084	29.23026141761225	40.95257137446708	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.15605797851109	37.81545658421881	31.18720384166569	s
44.95445973475206	42.77010767799165	47.09470807392681	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.00404363777253	44.71594251847980	45.26432009339950	h
46.90904869854552	39.34893612914239	45.54344481747887	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.81239164234332	33.36165818770797	41.32285300304112	s
44.19570272373237	25.90233700911505	42.11857291486434	n
46.09397798791569	29.61038858632800	45.51759906230516	s
40.35842460967742	25.30785146182419	41.42018898522077	h
40.24772735641245	28.42021736970910	44.68713849153652	s
39.63603687204049	33.91230556452197	45.71276084184398	c
37.82479286836904	35.13659585898142	45.81525560485284	o
44.44404444303773	34.90544253120506	46.71317901325223	c

45.62297319418266	36.67075379648725	47.38524312003535	n
41.93766215072497	31.51357750282442	49.15082118590198	c
41.35256917058384	32.48810874921414	51.05893131801223	o
40.07984392667024	26.92140128865273	49.95803445261254	c
38.25905905750573	26.22375415239940	51.02495422167566	n
44.95473687859727	28.00528317552564	50.74767854565576	c
43.55464191244080	24.40094756783755	47.38064733320191	o
44.61057743705942	22.84315363551273	48.96737100234840	o

Table 20: $[FeFe]_{Red} - O_2$

40.03137674922685	39.92622989962331	29.65877047340908	h
50.18995980804474	38.71724472752360	52.88471252838330	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.72196807645344	37.16193038853057	31.47296316786396	h
37.17136039439593	20.97207059528131	48.91501012215765	h
32.38265552592385	20.71924529171854	50.75796363378731	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.18465663282817	44.91188738253567	49.75523380354765	h
47.92348184100836	26.79865864964242	42.73137767054718	h
46.97509482574713	42.92131880468777	46.34784491187516	c
47.71568720249179	40.89927017202290	44.76846644160383	o
36.34203004003643	30.50027588105878	40.14711443756067	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.06632786006809	27.72765111240847	42.78636417249270	c
41.60495718703449	26.86209543149591	42.17578135854894	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.44915826611255	19.27743921277294	41.67703053299646	s
42.46586740275413	32.22667437756196	45.82490722937369	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.90019217376810	27.96309524614101	48.41960362000047	fe
37.06248146815346	37.12390955951309	38.44762170292162	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.56411543555271	26.44493899716518	34.08190858293169	s
39.30295804763396	33.39836864084674	38.68989837758601	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.18588284625601	30.23084825077466	35.97899073498485	fe
33.97908140842522	33.99293542113377	38.87490212925194	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.14680848443826	20.91253671552050	51.43968854812319	o
42.81154623250195	37.78411299999293	42.55218335398568	h
40.54674419785133	21.97402849158900	56.13458846736822	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.10256623448760	24.75706765957903	44.14512938539732	h
47.56267658359382	39.42222241983566	49.52670133163348	h
50.68712194190371	43.49383364699394	48.01499260272583	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.80006476449314	24.73617895500084	57.15960451011777	h
36.64045285493047	35.37360672016348	34.64064216379126	fe
41.18669145538884	21.19516248068403	45.21960644395352	h
41.65289885560409	17.91283573309368	45.66449614606988	h
43.84137066999730	21.82648205743217	41.46431394242330	h

39.84714671064681	32.34173746328113	34.62600970392599	s
32.93609170506035	32.99407000146832	34.95989260648973	s
46.23488912189914	27.85608670567731	52.80322976625305	o
39.19675152969939	25.22549059005098	36.69762586475506	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.92300279609690	22.59247914035918	35.01279859455907	h
34.52287390621140	37.53411343891430	43.23959415090927	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.83458739361686	35.56745751289998	41.25398543874691	s
32.00946411056986	37.13941824491658	45.43011127185050	h
33.61175282211438	28.73098831462652	44.86692837576941	h
35.69087333815993	29.67135506308873	47.33272309591852	h
32.57169470326289	24.95176385178339	47.87783145211205	h
35.43385839265916	25.82400537712041	49.34883241111043	h
35.44584634587320	25.01498093890367	46.34785322774466	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.34361811697132	25.91071822441361	47.66742901181712	n
34.73531772486756	18.73551817812734	48.18473725199544	h
37.42199907389149	24.56771275096218	54.24540281426894	h
25.19751707901032	20.41465586089941	46.93724680661799	h
24.75167751676310	21.22542275228264	50.15037909134371	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.46296103871713	22.15104792624831	48.67387796978773	c
29.47779802969744	24.20208427323042	47.98095088824076	o
29.53345285467660	20.22085196212824	49.59919660375881	o
45.90543146849832	36.50893223418596	42.22116702077263	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.57556176251045	28.21186225918131	40.59363482905416	h
45.92085386778089	29.10561619086319	41.23425947619906	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.14784048539122	37.90147989445966	31.16954031854955	s
45.00225024598328	42.68768398248794	47.00929330361460	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.05169902084607	44.67825183219807	45.22211463767403	h
47.00386861879096	39.30710849231917	45.52131862183781	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.76273967420125	33.37586291296081	41.30215343357284	s
44.11329084716843	25.83472974060832	42.51809821798632	n
46.09772879894092	29.60244035531682	45.79394488996916	s
40.27792393553976	25.32812411986928	41.73448437045532	h
40.19070721197831	28.50077661284479	44.96431617163058	s
39.70964316448772	34.03562679891810	45.94532220767983	c
37.88767890004812	35.26497001309085	46.06278352312577	o
44.49618546033872	35.01127638014391	46.81411883240002	c

45.69930708593905	36.79746317850633	47.41998221974091	n
42.04792770494699	31.49846152073575	49.38585664027219	c
41.51475192411380	32.58256255629234	51.27335720376969	o
40.03517874847370	26.96351105791420	50.24394059605839	c
38.16941708882451	26.28249214645246	51.26277792073112	n
44.91633897416630	27.87514785120784	51.03744312315830	c
43.33813321472746	24.30106535854596	47.52758168343119	o
44.80433055899515	22.74302336760405	48.83024592083654	o

Table 21: $[FeFe]^{\mu}_{Ox}$

39.94757438515317	39.94387356213088	29.64923234442961	h
50.19097031879298	38.71681582444723	52.88552204309801	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.76464881363966	37.21315843085436	31.45995855177068	h
37.17107994806837	20.87998367676424	48.77476600634485	h
32.47527447386648	20.90857458964575	50.83827399119436	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.23158740545367	44.91300431745772	49.77024452108975	h
48.16632090274503	26.77143342373707	42.69103977605879	h
46.91791082950392	42.95345233019520	46.39042229637241	c
47.58555538523696	40.92609405349568	44.77241214640722	o
36.37028074956476	30.51593939117901	40.20835247785104	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.30353940506631	27.68801874245560	42.69687367547321	c
41.86199919755394	26.80844060018597	41.92835632465583	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.58516297106772	18.97735966059592	41.85882029749033	s
42.66540951304385	32.10580142448726	45.48577367116378	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.08643546192769	27.50494963510640	48.25871840083317	fe
37.10945809398835	37.10493374040804	38.45673122923793	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.56091974395554	26.47448993892868	34.12432422703426	s
39.31203636563270	33.40019063599296	38.72811923243509	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
34.01069112356608	34.00969700854412	38.89291841867746	fe
36.20305756819735	30.20099554819827	36.02396326848942	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.27796792551818	21.06295719128393	51.43541125614128	o
42.92107982062498	37.85104613401398	42.58659821082257	h
40.55177806286778	21.97638686991402	56.13638466438162	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.40344038359476	24.54161047060078	43.67553552943316	h
47.59125134823020	39.41563648904798	49.52865118930114	h
50.67507458732208	43.46924148841997	47.97097073450458	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.75479973311641	24.67420661693496	57.13487785863926	h
36.67292521615128	35.32828863505391	34.62796816103666	fe
41.17698854717629	21.25573888383586	45.08259831752678	h
41.55795993209363	18.01456228088024	45.79235973293478	h
43.52428895304562	21.35938698441508	40.91263920302774	h

39.84422255496202	32.30198185455116	34.70137369801804	s
32.98131529054312	32.96986772606885	35.01531404788701	s
44.97192259173102	22.33564804391077	48.56028705026737	o
39.21409952142705	25.20257471074044	36.68135554776269	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.88502973956133	22.60138764694585	34.98572244044804	h
34.52787457634366	37.54666315996590	43.26081834408011	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.87164252324618	35.55517052256224	41.23952636500981	s
31.97740845645877	37.13201353316357	45.41884327561068	h
33.65341170803219	28.82703625555961	44.86828180185289	h
35.72017964477922	29.57870656878132	47.42937557157018	h
32.33960709713703	24.97715584392226	47.74546845457557	h
35.25447931389511	25.66147813237704	49.23488376806490	h
35.23110502777362	24.94152007134264	46.21302640504728	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.19251441060349	25.86280006360916	47.56272976838709	n
34.62717252475422	18.70243676280947	48.28395042467151	h
37.35183399926485	24.44866762733303	54.22450454128057	h
25.24506525866121	20.42992886753067	46.91137375263438	h
24.74974352479390	21.19460121251243	50.13454404515027	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44961870225784	22.23801608001154	48.68548202108197	c
29.41504217772137	24.25568553244464	47.80970251710158	o
29.58578889984594	20.44355852777798	49.77770698054346	o
45.92201734566825	36.42426832879956	42.17206582920247	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.79802494317349	28.20181001281354	40.38627572211429	h
46.22264371623558	29.16246637929394	41.23577639391403	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.16112264409662	37.80279431540961	31.20160210728468	s
44.95737721125589	42.74923789521419	47.09697824820888	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.99423545569216	44.70539624810819	45.26253237399334	h
46.95933320194218	39.32758205340356	45.55817084144213	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.60016850575512	33.44938861979472	41.50236220288267	s
44.38882841432403	25.81573555772209	42.21149455843855	n
46.17732355267537	29.43464837872463	45.81236456483970	s
40.55303885825788	25.26315163197430	41.46924633334180	h
40.49834268231263	28.39061674956972	44.77070694785105	s
40.15618476662372	33.43557754492905	47.21831900213851	c
38.53107060095834	34.37207752656168	48.37547128350414	o
44.62879494984033	34.85815590233639	46.72190207018259	c

45.78679178311585	36.63679643203254	47.42056780716733	n
44.44748406117507	28.65249734402447	51.08525020989363	c
45.30841742844269	29.32854786587638	52.99407638801467	o
40.06615922414726	26.76102551240369	50.00460956718640	c
38.17570481697142	26.19747124057551	51.04379157988026	n
44.16089341064031	24.38999934898510	48.35043203384059	c

Table 22: $[FeFe]^{\mu/Lys}_{Ox} - H^-$

39.93948339496662	39.94469525276106	29.65061041272790	h
50.18753515644907	38.71727033734878	52.88759695985596	h
50.26532597612761	40.64384966141100	52.02713464999426	c
51.72791730508891	42.27462094631834	52.76220787699877	o
40.76504260777251	37.21759784001318	31.46086889431643	h
37.12600723542798	20.88614565726514	48.72349673648577	h
32.51057114082706	21.00180055153358	50.88466524676957	h
48.55707969954778	40.96887121655315	50.21873477851589	n
48.71770075099387	43.22511728239375	48.64276366150725	c
48.25362452735596	44.91461040066916	49.77548734767564	h
48.11883629840435	27.06996449970432	42.25156250577650	h
46.89744657326310	42.97694670077284	46.40366183132426	c
47.52329102961721	40.93870511356003	44.78121607832273	o
36.38470038016159	30.61638889065315	40.17960957462881	s
39.24105115677064	18.94452330032199	43.50905052240016	h
46.22803537449420	27.91916671974471	42.35616651613825	c
41.77269316856113	26.82346713506423	42.03053392256741	c
41.12452228829050	19.35004718838886	44.26890561780783	c
43.58488368074904	19.12359044693884	41.84647059717314	s
42.55304599921801	32.21990505763277	45.50429957402246	fe
36.36718023232001	23.76148999498827	37.77248262407600	h
43.38635698406541	28.16490409669979	48.14686651464378	fe
37.15428801217669	37.12182331256668	38.40864944514678	s
37.43969996373850	24.30660984163455	36.08670897057459	c
35.60617318643142	26.51904235761548	34.13320184342597	s
39.33084351899059	33.42593804791368	38.75027953237237	fe
36.89179466078398	18.18345311101594	50.71280934307384	h
34.05765876400448	34.08317975245841	38.87952126667342	fe
36.24837787941688	30.23211686040264	35.99935996554277	fe
35.78436412893236	19.64294339940612	49.74701000483825	c
34.32227708183861	21.03549231864609	51.49390567447793	o
42.85760202890791	37.80823433515327	42.57023008146829	h
40.55338925242471	21.97990219532421	56.13525312397146	h
38.98732518887225	22.68717502375104	57.35097313453696	c
38.83615087832501	22.33192163006125	59.63556509225246	o
44.60313654478329	24.59920825083274	43.40381053088377	h
47.55828189235109	39.42719492841660	49.54463861917236	h
50.67055110431050	43.45620295395945	47.95499079732714	h
37.24884518401865	24.02694171349225	56.12459001229536	n
35.76139593311585	24.69172366312235	57.13206695567821	h
36.71374609345237	35.32397209653939	34.57416688058890	fe
41.13403209069516	21.21166828775043	45.17400616278687	h
41.59655210561928	17.94235515278054	45.71362553405361	h

43.09319183437926	21.32629824742953	40.63927773783909	h
39.87872488194424	32.33085394342898	34.72408228619731	s
33.02735058248076	33.00484961397502	35.03187282321206	s
44.88577381559034	22.87068579114197	48.10641441820657	o
39.23122895517002	25.16627747874725	36.68095786698267	h
31.89727118913942	39.64356849057265	43.16713103624832	h
37.85058538612586	22.60746015160059	34.96334938466826	h
34.53142852678439	37.53631424100624	43.32971744811068	h
32.47179895374285	37.67779411713094	43.47525088092853	c
30.92573350235651	35.59421287177701	41.17171728725341	s
31.91655312583600	37.09753636164950	45.38987975075757	h
33.55113223358790	28.83555986760570	44.87543020772552	h
35.64294829141803	29.75465034926594	47.33328722096963	h
32.83470527126294	24.87906292858138	47.51202326960167	h
35.55611081244687	25.71109403707821	49.05317221253159	h
42.49004385572996	31.29088305708330	48.46209287230457	h
32.35447908672487	29.36437866723039	47.94215148011812	h
33.97407453132900	28.60368075397097	46.89930233858816	c
34.46006833934726	25.97313394949846	47.48350857240768	n
34.58944862558472	18.70136710639524	48.31303631043900	h
37.43442188881129	24.57159552920441	54.26569002556947	h
25.25787187652953	20.44855408604915	46.88531779895079	h
24.72334934817718	21.17359145426583	50.11550738563114	h
24.62496255328159	23.63589501726895	47.76380857707185	h
25.56800391979389	21.88976918051362	48.35626795287534	c
28.45011274163901	22.24893551367960	48.69469871797682	c
29.41573053509823	24.13488385250753	47.61453331057351	o
29.55266479220187	20.55809657673518	49.99526050781532	o
45.91305963914838	36.47403495778472	42.19956654907908	h
39.60187168362467	36.84896401816100	28.32450962379954	h
41.48006167297021	28.14649908404529	40.45169284127243	h
46.00164614565401	29.31727894624533	40.83284807300667	h
39.43517138323448	37.96880060202321	30.05871317843228	c
36.15334094836778	37.79221633285508	31.18101386753246	s
44.93950318631563	42.79935360403731	47.12334446617745	h
44.15765555110334	37.44255722963949	39.48606548723281	h
46.99173944116786	44.72739123956730	45.27486832169980	h
46.86997297730223	39.35831827958591	45.57948768173015	h
44.02135905433818	36.58935344310939	41.36828939951017	c
42.71584935922142	33.41274007889951	41.39482215675966	s
44.35862965895007	25.96888861886783	42.06205039311082	n
46.25233360385369	29.84009570561622	45.34439988411901	s
40.50496435869987	25.20066481665441	41.76263192304306	h
40.51986000614641	28.45806903773501	44.89664959976161	s
39.76425667196768	33.85545691389378	46.16730533045008	c
37.94885907328519	35.01593960633501	46.60353707955152	o

44.46124138996854	34.98922871797997	46.76448970598865	c
45.61662724383638	36.75207039520783	47.49990142172827	n
45.25339576598757	28.90722641625502	50.80722639406137	c
46.43512907907333	29.37150059023055	52.59432562796914	o
40.56442029624771	27.40338681469021	50.25326477984309	c
38.85107323142753	26.79548561262401	51.52093614248016	n
44.26011239074516	24.98384067181653	48.07583029603271	c

Table 23: $[FeFe]^{\mu/Lys}_{Red} - H^-$

39.97848847285012	39.93366546430765	29.62233702944390	h
50.20146726426356	38.70847761376294	52.86715451793533	h
50.26435654662549	40.64306542506912	52.02613120542189	c
51.72691952969490	42.27380458463235	52.76118931461740	o
40.78549292836497	37.20678736193276	31.43478063058643	h
37.09692111142125	21.00147142165944	48.84544974532167	h
32.40409109218679	20.82461393841862	50.83637440654947	h
48.55614239538979	40.96808131103290	50.21776534901377	n
48.71676155710975	43.22428391317263	48.64182446762312	c
47.85643041192647	44.86024277569251	49.61752617987052	h
47.72478077243959	26.46213670508689	42.31870898778946	h
47.36849706190113	42.73680591802827	46.12105282279415	c
48.50956669887366	40.75928037922309	44.72594268706199	o
36.30389890917148	30.55535378947218	40.29861030336323	s
39.24029337659451	18.94415858317986	43.50821148400066	h
45.92911810960333	27.48165135659545	42.54295946436704	c
41.37973303551752	26.77858454628515	42.66664461120914	c
41.12372860331800	19.34967302261611	44.26805146159933	c
43.54050251862381	19.26258013935294	41.77411660088434	s
42.93842687237867	32.31185819973874	45.61736218343430	fe
36.36647914392764	23.76103079153990	37.77175318979175	h
43.60430123685996	28.36939163531935	48.48336182302478	fe
37.29505474835396	37.04916557364626	38.61943514394710	s
37.43897808835875	24.30614118955555	36.08601355136059	c
35.51387228213073	26.45978870187153	34.15798463419773	s
39.27944765389142	33.40755681902133	38.91711376841454	fe
36.89108223403486	18.18310162195669	50.71183046494110	h
34.14713250381133	33.96839024104522	39.08826156978326	fe
36.82072513007288	35.23447950576508	34.63650611447934	fe
35.78367437889674	19.64256356445499	49.74605002396675	c
34.19564314879060	20.84628724708873	51.52527539075699	o
42.70655033797810	37.71864779520583	42.50233988989922	h
40.54862647793521	21.97455177713059	56.13341493133890	h
38.98657307787450	22.68673660729004	57.34986575502771	c
38.83540065705339	22.33149077250475	59.63441424904233	o
44.10795217908052	24.59678394507041	44.23008988404171	h
47.63846811943269	39.38802004243279	49.47821526708203	h
50.72110480000521	43.68067838363915	48.31098306864106	h
37.24812708809115	24.02647873059162	56.12350719922574	n
35.79701387246877	24.75706195018389	57.13837391000521	h
36.11802398907720	30.27495239241157	35.91818844458921	fe
41.10155811220557	21.19144047269808	45.21004047689613	h
41.61536312403389	17.92296221624905	45.68746747206255	h

43.62599834799610	21.80850589914332	41.30733238368329	h
39.85326011650966	32.30085144513731	34.69021817205375	s
33.09655691157339	32.96483812051397	34.93700345356464	s
44.39149321710337	22.92955882812053	48.79397130576868	o
39.20056313265410	25.22246557119895	36.68577141816336	h
31.89665513842268	39.64280315149202	43.16629766702720	h
37.90156896988292	22.60174707439170	34.98745072557423	h
34.52909243839440	37.53691360351384	43.27970297238381	h
32.47117156466935	37.67706657257282	43.47441184252903	c
30.83977753054680	35.66801248159206	41.14618811444057	s
31.95222246093666	37.08701948497776	45.39649523906001	h
33.42734095067499	28.49675151526558	44.89270791084607	h
35.53355458764219	29.96548268293675	47.00963618521003	h
33.29870203528774	25.09052291732414	48.42281673713602	h
35.94870311767399	26.35107944822806	49.35848275798104	h
43.02282240517903	31.58296688901769	48.62993377988077	h
32.35385547710363	29.36381174939289	47.94122551431688	h
33.97341879636362	28.60312895394247	46.89839715977428	c
34.82658713330978	26.11142944095490	47.80256410546686	n
34.69002138416734	18.72755696285602	48.21573422150455	h
37.52158638775953	24.71802432976270	54.33183393505821	h
25.64908654265324	20.56512047389219	46.75178655472907	h
24.41871579912960	20.97886787549494	49.83987869435973	h
24.62448823202422	23.63543959327282	47.76288639072285	h
25.56751070127527	21.88934588186162	48.35533442816959	c
28.27425236879723	22.34671936696135	49.41348893329131	c
28.88487471243772	24.56099592577582	49.95637646436030	o
29.57728347713199	20.32491236337847	49.65096320143454	o
45.88550966476514	36.64640003023136	42.25955792122588	h
39.60110823427016	36.84825348113800	28.32396349294942	h
41.10390829604152	27.96620005684706	40.98335801420593	h
45.64027921020116	28.76438511398155	40.93107837342776	h
39.43440982360611	37.96806738828671	30.05813303251191	c
36.21102185264654	37.87253962348848	31.32310974378971	s
45.34611859827496	42.33527523925373	46.48018441280091	h
44.15680328462096	37.44183535425974	39.48530392760443	h
47.46456211006448	44.47406348854097	44.96864534619547	h
47.83705088385661	39.14081229853198	45.44398352515678	h
44.02051056730805	36.58864668553863	41.36749193508542	c
42.96081012539845	33.31829776646855	41.35162066817927	s
43.88574392484495	25.67040897632598	42.63411857019846	n
46.39384172412854	29.59340757861465	45.35021903129765	s
39.95176321418387	25.27211408400756	42.64624078731588	h
40.52911718874084	28.77449909604951	45.42658797946211	s
40.32538024847679	34.20703578190983	46.26196005517764	c
38.63822930471569	35.55480133547201	46.68730737554528	o

45.07511752941775	34.97904343045398	46.66806825541963	c
46.32705189312887	36.70098552098314	47.35743399492046	n
45.76753274128069	29.03280356434010	50.92586596411891	c
47.15798123599395	29.42183370340975	52.58441971785266	o
40.89769357938544	28.05408496869080	50.84716423516058	c
39.25370831645998	27.70191856306326	52.29329404298353	n
44.05918453380023	25.10443954594511	48.60357431477597	c

Table 24: TS1

39.84829934403287	39.96361755706840	29.62978730966338	h
50.18591007743154	38.71873117052284	52.89006358194013	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.82994598081154	37.27570473164602	31.42885708155292	h
37.16955477031578	20.96337660770191	48.88998403171016	h
32.40345574685137	20.77898539271229	50.72198791993929	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.26327425921912	44.91752291937863	49.77748611616052	h
47.97106971388735	26.69155790676997	42.93361497791965	h
46.88974687908851	42.97604624939709	46.41094767665032	c
47.50827530420457	40.93074649875290	44.79789236024416	o
36.39856645036316	30.47958438330307	40.25304414506082	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.16530315750850	27.71204639084376	42.91593157138467	c
41.62883524103550	26.83672889352108	42.28803925172359	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.33495827995488	19.56182937966541	41.59305248130088	s
42.47041583478661	32.27898259174142	45.56264529141549	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.04151705945016	27.95958963993476	48.16636146638308	fe
37.16233291629239	37.18436657368471	38.49466415144827	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.63216628802412	26.57762282486271	34.17342573944013	s
36.77173470845845	35.25788104188769	34.79225656287650	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
39.22708126943234	33.42853767297574	38.75090224148494	fe
34.17820889092567	34.00324674455839	38.86693775577350	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.16636414577427	20.94167171325365	51.42721891417174	o
42.83144336862907	37.80646392915461	42.54825501401444	h
40.55514062406705	21.98613940816390	56.13574220014182	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
43.69849045191054	25.79458732682770	45.70770279603076	h
47.54380263062883	39.43144882584294	49.55262056817807	h
50.66958236369496	43.45113043629196	47.94799750100827	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.73104356478628	24.64494785489418	57.11660590757051	h
36.32252581000661	30.32320377789231	36.09898344659439	fe
41.10846132323695	21.10407254663674	45.37635056258422	h
41.75650087865858	17.78486519513826	45.46638742371021	h
41.78271104527856	20.85288709018763	40.01953744373679	h

39.99884020535678	32.32603146225736	34.78552463760287	s
33.06405306077715	32.97333569890255	35.02643625482227	s
46.21945678515969	23.72756747583476	49.68013471678533	o
39.25019372670472	25.13109016941171	36.68862675055837	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.82192294761217	22.60489287318266	34.95227347370523	h
34.53619729906014	37.55672871432844	43.35941653174974	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.98413242798326	35.56657610334231	41.15271978039193	s
31.90012015453701	37.10879799814437	45.39114699821454	h
33.66447960278835	28.85329804868771	44.86987097433039	h
35.71604640507511	29.57749511337067	47.43917035706474	h
32.34457446406109	24.98794287721837	47.80348371429187	h
35.36654761401817	25.59059065207613	49.12702749586219	h
35.12494085223050	24.93219402668007	46.10518660890285	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.19724467408184	25.85259709164615	47.53261315550949	n
34.71592602278061	18.72189221198038	48.20486871459076	h
37.35154610778761	24.37319462546068	54.20806703424927	h
25.18233241239653	20.39721197622397	46.96217763212741	h
24.79335315411705	21.24627833873744	50.17442356295138	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.45865799077050	22.19838657648126	48.61431491051044	c
29.41079674319019	24.29848568412529	47.94474775645554	o
29.61643159369035	20.29095008659575	49.46992275997652	o
45.90957018219376	36.50867402965380	42.21450252551195	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.71185502446448	28.05923629087219	40.60917123058727	h
46.01049873273807	28.90567972232135	41.21750760692863	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.20384383396193	37.64063984827612	31.28195555695823	s
44.93414212651449	42.80422279097819	47.13781136214458	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.98336816734313	44.72399684473255	45.27707111071062	h
46.82343493624294	39.35792130383727	45.58961498460253	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.72495091747607	33.39690362250300	41.41299158584707	s
44.10445723468685	25.87315935253779	43.04624470476119	n
46.10110212307683	29.87310720533634	45.67685006963633	s
40.35789724634256	25.23928287110416	41.91124311049585	h
40.26725201962095	28.70329970918223	44.92346462746862	s
39.75219079587917	33.97020196493465	46.30683970358658	c
37.96765581860741	35.15861042457336	46.82747587433468	o
44.39579987408755	35.01502757787551	46.84684158713676	c

45.56774938709323	36.78442755809098	47.54707382455297	n
43.31503517897659	30.33950514147714	50.54023348502563	c
43.57525962910880	31.64663299777555	52.29229607338117	o
40.22644747444499	26.55338132277916	49.80942058873624	c
38.42870099435765	25.67502380945140	50.79936159509150	n
44.93904307940139	25.44720181667234	49.10057469197847	c
44.52679827777226	24.13572509807189	42.28494026975803	h

Table 25: TS2

39.97865174374265	39.93731532486163	29.65429460609664	h
50.18843010855773	38.71769197638795	52.88794213763953	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.74612056759177	37.19345977894047	31.46688644404880	h
37.17385869077192	20.85489858064904	48.74869094184101	h
32.49160240669912	20.93937281039560	50.84786205149346	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.23965527666119	44.91568615184489	49.76964539954728	h
47.97234642834242	26.55985751619524	42.84347925242682	h
46.90817696665798	42.94789419023849	46.39785290808341	c
47.54744071914269	40.88572448071459	44.81426450122440	o
36.32343326396328	30.50626642325350	40.16819917773834	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.14326963972891	27.53416293705264	42.73328908365374	c
41.70382110810864	26.72985974887630	41.86844798060197	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.54969168195408	19.09834777106111	41.79571164305204	s
42.48811294105116	32.19052953790662	45.42040636730196	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.74166737172849	28.01086698686054	48.03246963545078	fe
37.05728849898718	37.15442174784690	38.44741130514755	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.57118659991237	26.47715019536808	34.11374270628910	s
39.27915662972293	33.43611930038241	38.71225222459121	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.19027418152164	30.23484339694422	35.99825686977099	fe
33.97409522758412	34.01787191991041	38.87722017334694	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.30051355500881	21.10585343316099	51.42068016982409	o
42.76107594644562	37.75012607516815	42.53046782856814	h
40.55591105923971	21.98381800512867	56.13695202761792	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.02552963711350	24.67287869314555	44.07696292504043	h
47.56146798983145	39.42657267037944	49.54892916323872	h
50.67361176083042	43.46162641450727	47.96445948674216	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.73450793369262	24.63684723753866	57.12802365466696	h
36.64251584369682	35.38202187392091	34.63692894917126	fe
41.14777008144270	21.23956031651585	45.12326016613065	h
41.57210327100839	17.98047704505903	45.75839707095950	h
43.84803977518175	21.61853787133131	41.33099665800676	h

39.83990879991219	32.34729885288606	34.68897067100730	s
32.95922800615784	32.99196963523314	34.97844764113832	s
45.52422625005779	23.32544107982098	49.07924023595790	o
39.21501039191160	25.20006352876374	36.68271053138274	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.88800302442015	22.59807521762561	34.99142194191013	h
34.52555772483527	37.53705098345728	43.25043716874879	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.84244387907968	35.54826547152987	41.26608651867139	s
31.99683107274228	37.14283445325182	45.42720760165241	h
33.68981664584329	28.87350299048328	44.86834631599958	h
35.71708704178241	29.56089024826803	47.46725877653641	h
32.22590272840664	24.97100422249991	47.65311058598081	h
35.11474312343308	25.51511104362114	49.18453489217707	h
35.15074897218294	24.91818905910277	46.13806044143969	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.13050619510243	25.83589508410338	47.50471905395847	n
34.60795184086918	18.69603270570966	48.30411741219488	h
37.34315178191608	24.37632905345768	54.20878873205867	h
25.24636888080051	20.43112164573877	46.91051881228734	h
24.75971515724751	21.19400962254141	50.13779940807272	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44851305239830	22.25012654374587	48.67192316374722	c
29.40726741762135	24.25199192562899	47.73601485591571	o
29.59713823810964	20.49490592529306	49.80617589464384	o
45.89696996837704	36.56598028524004	42.24141546839957	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.78911266899381	27.98404331128409	40.21114313509258	h
46.12857652979363	28.84413260899615	41.11695332184325	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.15388247880404	37.84221692200480	31.18131647469903	s
44.94693754186137	42.77924423995321	47.10998737703732	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.00614990792742	44.68238669683380	45.24455361139961	h
46.85314160106535	39.31489027409857	45.59923305087332	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.84743130163695	33.36173008941671	41.29462983368182	s
44.15648328607020	25.67668754694955	42.41447519225899	n
45.99573158201390	29.61175753374264	45.60463560477915	s
40.34140332147713	25.21282620770969	41.48665314492688	h
40.22640736825477	28.70086187179109	44.40759036526896	s
39.78136320475536	33.91008039465311	46.14562472769379	c
37.99959806595682	35.09669202300039	46.68042734415003	o
44.43084623626808	34.89380998819619	46.75368576484757	c

45.59410933682964	36.65839780158321	47.47810817036445	n
43.32175843137615	30.43238756618086	50.31298925868628	c
43.70897792219321	31.75413568553317	52.02859235790731	o
40.10176555820653	26.65054534419199	49.99707621704196	c
38.38944799013868	25.73910275376953	51.11688425578356	n
44.39628110549216	25.15945507207774	48.57105666940747	c
39.81867446083634	27.89900030317419	47.82747594831807	h

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