Electronic Supplementary Information (ESI)

Water Formation on Interstellar Silicates: Role of Fe^{2+}/H_2 interactions in the $O + H_2 \rightarrow H_2O$ reaction

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Table S1. Lattice parameters (*a*, *b* in Å, and γ in degrees) of the B3LYP-D3(BJ)-optimized surfaces for the Mg_2SO_4 and (Mg,Fe)SiO_4 systems.

Surface	*a*	*b*	γ
(010)-Mg	4.78095	12.16320	90.07227
(010)-Fe1 Q	4.74823328	12.08573786	89.999270
(010)-Fe1 T	4.74514896	12.09325602	89.986586
(010)-Fe1 S	4.74750442	12.07195125	89.956311
(001)-Mg	4.75996	9.78703	91.60683
(001)-Fe1 Q	4.76836083	9.78889719	91.673278
(001)-Fe1 T	-	-	-
(001)-Fe1 S	4.75630825	9.77261366	91.788967
(001)-Fe4 Q	4.76946787	9.78397288	91.713665
(001)-Fe4 T	4.75818705	9.78456149	91.490428
(001)-Fe4 S	4.75298384	9.76232226	91.399307
(110)-Mg	5.72247	11.29350	91.71496
(110)-Fe2 Q	5.73526375	11.34338253	91.731749
(110)-Fe2 T	5.72251573	11.33914547	91.811724
(110)-Fe2 S	5.78335657	11.28458030	91.688910
(110)-Fe8 Q	5.73563564	11.36520956	91.718696
(110)-Fe8 T	5.75680944	11.34386635	91.782465
(110)-Fe8 S	5.70216835	11.37243813	91.786953

Rate Constants Description with Tunneling Effects

The classical rate constant is given by the Eyring equation [1]

$$k_{classical}(T) = \frac{k_B T}{h} e^{-\Delta G^{\ddagger}/k_B T}. \tag{A.1}$$

In general, this variable is represented in an Arrhenius plot: $\ln k$ vs $1/T$,

$$\ln k = \ln\left(\frac{k_B T}{h}\right) - \frac{\Delta G^{\ddagger}}{k_B} \cdot \frac{1}{T}\ . \tag{A.2}$$

In order to include the tunneling effect, the semi-classical rate constant is defined as

$$k_{SC}(T) = \kappa(T) k_{classical}(T), \tag{A.3}$$

where $\kappa(T)$ is the transmission coefficient that depends on the transmission probability of the tunneling effect [2]. The analytic expression of this coefficient is different depending on the potential barrier approximation used. However, its general equation is

$$\kappa(T) = \frac{\int_{E_0}^{+\infty} P^T(E) e^{-\beta E} dE}{\int_{E_0}^{+\infty} P^C(E) e^{-\beta E} dE}, \tag{A.4}$$

where $\beta = 1/k_B T$, $P^T(E)$ is the quantum transmission probability, $P^C(E)$ is the classical transmission probability and $E_0 = \max(E_r, E_p)$ with E_r the reactant's energy and E_p the product's energy [2]. It is very important that all the energies include the Zero Point Energy (ZPE) and they must have the same energy origin.

The Variational Transition State Theory (VTST) states that the classical transmission probability is given by

$$P^C(E) = H(E - E^{\ddagger}), \tag{A.5}$$

where $E^{\ddagger}$ stands for the maximum energy of the potential barrier and $H(x)$ is the Heaviside step function [2]. Thus, the transmission coefficient results in

$$\kappa(T) = \beta e^{\beta E^{\ddagger}} \int_{E_0}^{+\infty} P^T(E) e^{-\beta E} dE. \tag{A.6}$$

In the next sections, the following 1D potentials are studied:

- Asymmetric squared barrier
- Asymmetric truncated parabolic barrier
- Asymmetric and approximated Eckart barrier
- General potential barrier

In general, the uni-dimensional potential barrier underestimates the transmission coefficient because it does not take into account the curvature of the reaction path.

A.1 Theoretical Description of the Potential Barriers

In this section, the potential barriers and their transmission coefficients are described. The characteristic parameters and some approximations are also included.

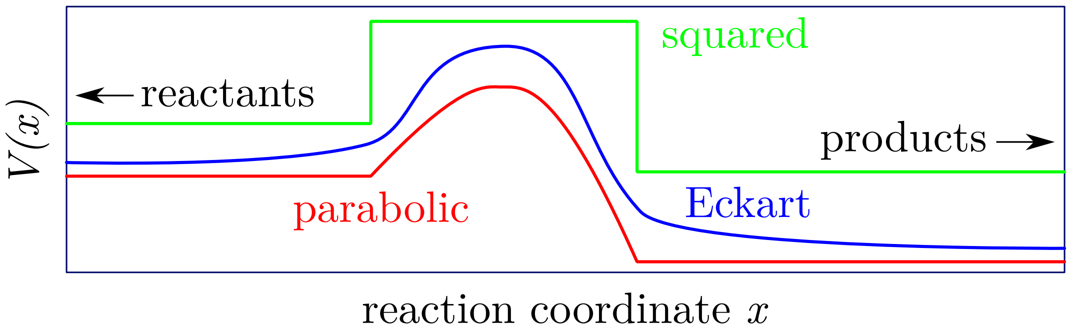

Fig. S1 | Symbolic representation of the described potentials.

A.1.1 Asymmetric Squared Barrier

Potential:

$$V(x) = \begin{cases} E_r & x \leq 0 \\ E^{\ddagger} & 0 < x \leq l \\ E_p & l < x \end{cases} \tag{A.7}$$

where l is the barrier's width. This parameter can be estimated from the characteristic length of the parabolic or Eckart potential:

$$l_{parabolic} = \sqrt{\frac{V_{max}}{2\pi^2\mu|\nu^{\ddagger}|^2}} + \sqrt{\frac{V_{max} - \Delta V}{2\pi^2\mu|\nu^{\ddagger}|^2}} \tag{A.8}$$

$$l_{Eckart} = \frac{1}{|\nu^{\ddagger}|}\sqrt{\frac{2}{\mu}}\left(\frac{1}{\sqrt{V_r}} + \frac{1}{\sqrt{V_f}}\right)^{-1} \tag{A.9}$$

where $\nu^{\ddagger}$ is the imaginary frequency of the transition state (TS), μ is the reduced mass associated to this mode, $V_{max} = E^{\ddagger} - E_r$, $\Delta V = E_p - E_r$, $V_f = E^{\ddagger} - E_r$ and $V_r = E^{\ddagger} - E_p$ [2,3,4]. It is worth mentioning here that some formulae in [2] are not correct). The nomenclature V_r and V_f corresponds to *reverse* and *forward*, respectively, and r should not be confused with 'reactants'.

Using the expressions of subsection A.1.4, it can be noticed that $s_1 = 0$ and $s_2 = l$, so

$$\theta(E) = \frac{\sqrt{2\mu}}{\hbar}\int_0^l \sqrt{E^{\ddagger} - E}\, dx = \frac{l}{\hbar}\sqrt{2\mu(E^{\ddagger} - E)}\,. \tag{A.10}$$

Then, the transmission probability can be written as

$$P_{squared}(E) = \begin{cases} 0 & E \leq E_0 \\ \left(1 + e^{2\theta(E)}\right)^{-1} & E_0 < E \leq E^{\ddagger} \\ 1 - \left(1 + e^{2\theta(2E^{\ddagger} - E)}\right)^{-1} & E^{\ddagger} < E \leq 2E^{\ddagger} - E_0 \\ 1 & 2E^{\ddagger} - E_0 < E \end{cases} \tag{A.11}$$

In order to determine the transmission coefficient, the following integral has to be computed

$$I \equiv \int_{E_0}^{+\infty} P_{squared}(E)e^{-\beta E} dE \equiv I_1 + I_2 + I_3, \tag{A.12}$$

where

$$I_3 = \int_{2E^{\ddagger}-E_0}^{+\infty} e^{-\beta E} dE = \frac{1}{\beta} e^{-\beta(2E^{\ddagger}-E_0)} \tag{A.13}$$

and I_1 and I_2 have to be numerically integrated.

A.1.2 Asymmetric Parabolic Barrier

Potential:

$$V(x) = \begin{cases} 0 & x \leq -\sqrt{\dfrac{V_{max}}{2\pi^2\mu|\nu^{\ddagger}|^2}} \\ V_{max} - 2\pi^2\mu|\nu^{\ddagger}|^2 x^2 & -\sqrt{\dfrac{V_{max}}{2\pi^2\mu|\nu^{\ddagger}|^2}} < x \leq \sqrt{\dfrac{V_{max}-\Delta V}{2\pi^2\mu|\nu^{\ddagger}|^2}} \\ \Delta V & \sqrt{\dfrac{V_{max}-\Delta V}{2\pi^2\mu|\nu^{\ddagger}|^2}} < x \end{cases} \tag{A.14}$$

where $\nu^{\ddagger}$ is the imaginary frequency of the TS, μ is the reduced mass associated with this mode, $V_{max} = E^{\ddagger} - E_r$ and $\Delta V = E_p - E_r$ [2]. It is important to notice that this potential has its energy origin on the reactants, $V(x \to -\infty) = 0$.

The transmission coefficient is found to be

$$\kappa(T) = \begin{cases} \dfrac{\pi/K}{\sin(\pi/K)} + \exp\left[(1-K)\dfrac{V_b}{k_BT}\right]/(1-K) & K > 1 \\ V_b/k_BT & K = 1 \\ \left(\exp\left[(1-K)\dfrac{V_b}{k_BT}\right] - 1\right)/(1-K) & K > 1 \end{cases} \tag{A.15}$$

where $K = 2\pi k_BT/h|\nu^{\ddagger}|$ and $V_b = V_{max} - \max(0, \Delta V)$ [2].

A.1.3 Asymmetric Eckart Barrier

Potential:

$$V(x) = \frac{Ae^{(x-x_0)/l}}{1+e^{(x-x_0)/l}} + \frac{Be^{(x-x_0)/l}}{\left(1+e^{(x-x_0)/l}\right)^2} \tag{A.16}$$

where

$$\begin{aligned}
A &= V_f - V_r \\
B &= \left(\sqrt{V_r}+\sqrt{V_f}\right)^2 \\
l &= \frac{1}{|\nu^{\ddagger}|}\sqrt{\frac{2}{\mu}}\left(\frac{1}{\sqrt{V_r}}+\frac{1}{\sqrt{V_f}}\right)^{-1} \\
x_0 &= \frac{l}{2}\ln(1-\Delta V/V_{max}) \quad \text{corresponds to the position of the maximum of the potential}
\end{aligned} \tag{A.17}$$

with $V_{max} = E^{\ddagger} - E_r$, $\Delta V = E_p - E_r$, $V_f = E^{\dagger} - E_r$ and $V_r = E^{\dagger} - E_p$ [2,4]. The nomenclature of V_r and V_f is the *reverse* and *forward* potential, respectively. It is important to notice that the potential has its energy origin on the reactants, $V(x \to -\infty) = 0$.

The transmission probability is given by

$$P_{Eckart}(E) = \frac{\cosh(a+b)-\cosh(a-b)}{\cosh(a+b)+\cosh(d)}, \tag{A.18}$$

where

$$\begin{aligned}
a &= \frac{4\pi}{h|\nu^{\ddagger}|}\left(\frac{1}{\sqrt{V_r}}+\frac{1}{\sqrt{V_f}}\right)^{-1}\sqrt{E} \\
b &= \frac{4\pi}{h|\nu^{\ddagger}|}\left(\frac{1}{\sqrt{V_r}}+\frac{1}{\sqrt{V_f}}\right)^{-1}\sqrt{E-V_f+V_r} \\
d &= 4\pi\sqrt{\frac{V_fV_r}{(h|\nu^{\ddagger}|)^2}-\frac{1}{16}}
\end{aligned} \tag{A.19}$$

as described in [2,4].

The expression of the transmission coefficient is

$$\kappa(T) = \beta e^{\beta E^\ddagger} \int_{E_0}^{+\infty} P_{Eckart}(E - E_r) e^{-\beta E} dE \tag{A.20}$$

because the energy origin of $P_{Eckart}(E)$ is different from the integral variables. For example, when in the integral $E = E_r$, then $P(E_r - E_r) = P(0)$ that agrees with the energy origin of the Eckart potential. Moreover, as the minimum value of E in the integral is $E_0 = \max(E_r, E_p)$, there will be no problem in evaluating $\sqrt{E - E_r}$ or $\sqrt{E - E_r - V_f + V_r}$ when $E \in [E_0, +\infty)$ as

- $\sqrt{E - E_r}$, $E - E_r \geq 0$ because $E \in [\max(E_r, E_p), +\infty)$
- $\sqrt{E - E_r - V_f + V_r} = \sqrt{E - E_r - E_p + E_r} = \sqrt{E - E_p}$, $E - E_p \geq 0$ for the same reason.

In addition, certain approximations can be done to simplify the calculations of $\kappa(T)$ [2]. Assuming that the barrier is symmetric ($\Delta V = 0$) and that it is very high or wide, in other words

$$\gamma = \frac{2\pi V_{max}}{h|\nu^\ddagger|} \gg 1, \tag{A.21}$$

then the transmission coefficient can be approximated to

$$\kappa(T) = \frac{h|\nu^\ddagger|}{2\pi k_B T} \int_{-\gamma}^{+\infty} \frac{\exp\left[-h|\nu^\ddagger| x / 2\pi k_B T\right]}{1 + \exp\left[2\gamma\left(1 - \sqrt{1 + x/\gamma}\right)\right]} dx \tag{A.22}$$

where $x = \gamma(E - E_{max})/V_{max}$.

Moreover, assuming also high temperatures (i.e. $2\pi k_B T / h|\nu^\ddagger| \gg 1$) leads to the analytical expression

$$\kappa(T) = \frac{h|\nu^\ddagger|/2k_B T}{\sin(h|\nu^\ddagger|/2k_B T)}. \tag{A.23}$$

Finally, this expression can be simplified in order to obtain the Wigner tunneling expression

$$\kappa(T) = 1 + \frac{1}{24}\left(\frac{h|\nu^\ddagger|}{k_B T}\right)^2. \tag{A.24}$$

A.1.4 General Potential Barrier

Potential: any $V(x)$ that fulfills $V(x \to -\infty) = E_r$ and $V(x \to +\infty) = E_p$.

This general barrier is a zero-curvature tunneling model (ZCT), which uses the semi-classical WKB approximation. The model is considered multidimensional if the potential includes all the vibrational ZPE in the orthogonal directions of the reaction path [2].

The transmission probability is given by

$$P_{ZCT}(E) = \begin{cases} 0 & E \leq E_0 \\ \left(1 + e^{2\theta(E)}\right)^{-1} & E_r < E \leq E^{\ddagger} \\ 1 - \left(1 + e^{2\theta(2E^{\ddagger} - E)}\right)^{-1} & E^{\ddagger} < E \leq 2E^{\ddagger} - E_0 \\ 1 & 2E^{\ddagger} - E_0 < E \end{cases} \tag{A.25}$$

where

$$\theta = \frac{1}{\hbar} \int_{s_1}^{s_2} \sqrt{2\mu(V(x) - E)}\, dx \tag{A.26}$$

with s_1 and s_2 being the crossing points between $V(x)$ and E. In other words, they are the points that fulfill $V(s_1) = E = V(s_2)$.

The transmission coefficient is then

$$\kappa(T) = \beta e^{\beta E^{\ddagger}} \int_{E_0}^{+\infty} P_{ZCT}(E) e^{-\beta E} dE. \tag{A.27}$$

The ZCT underestimates the transmission by tunneling effect because it does not take into account the curvature of the reaction path. In [2], several sophisticated methods are described, such as small-curvature tunneling, large-curvature tunneling, microcanonically optimized tunneling and least-action tunneling.

References

[1] H. Eyring, *J. Chem. Phys.*, 1935, **3**, 107.

[2] J. L. Bao and D. G. Truhlar, *Chem. Soc. Rev.*, 2017, **46**, 7548.

[3] V. Taquet, P. S. Peters, C. Kahane, C. Ceccarelli, A. Lopez-Sepulcre, C. Toubin, D. Duflot and L. Wiesenfeld, *Astron. Astrophys.*, 2013, **550**, A127.

[4] P. S. Peters, D. Duflot, A. Faure, C. Kahane, C. Ceccarelli, L. Wiesenfeld and C. Toubin, *J. Phys. Chem. A*, 2011, **115**, 8983.

Fractionary coordinates of the periodic systems

Optimized fractionary coordinates have been written in the MOLDRAW format (MOLDRAW is freely available at http://www.moldraw.unito.it). Each coordinates block starts with a TITLE record and finishes with a “ -1 0 0 0” record. The coordinates of each structure can be copied and pasted in an ASCII editor and saved as a file with .mol extension.

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 8   0.475304401218   0.190120471236   0.896536139986001
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 14   0.25615334543   0.091389856015   0.675562267197996
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Optimized cartesian coordinates of the molecular systems

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12	0.078162	1.164449	-1.686759
8	1.686579	0.024226	-1.913240
14	-0.221237	0.430502	1.719108
8	-0.056170	-1.100700	2.319429
8	0.815197	0.264340	0.385711
8	0.189186	1.853382	2.314695

NCl-Fe16_Q

8	1.606207	-0.187887	1.102411
12	1.277774	2.652738	0.430585
8	2.802716	1.740876	-0.277980
14	2.421235	0.197372	-0.482359
8	3.291478	-1.161408	-0.459973
12	1.982410	-2.109213	0.603354
8	0.222915	-2.673773	0.098934
12	-1.271468	-2.067274	1.256251
8	-2.802027	-1.558976	0.167803
14	-2.419602	-0.124184	-0.442332
8	-3.084212	1.289169	-0.073552
12	-1.533251	2.245663	0.607144
8	-0.255210	2.849974	-0.709634
12	-0.279054	1.282461	-1.810574
8	1.204660	0.033085	-1.618684
26	-0.190935	-1.464423	-1.301558
8	-1.653526	-0.195856	-1.944811
14	0.126495	0.238411	1.732573
8	0.071208	1.874898	1.918806
8	-0.830893	0.134472	0.328784
8	-0.441616	-0.937058	2.654029

NCl-Fe16_S

8	1.671084	-0.160456	1.083662
12	1.025715	2.715655	0.579038
8	2.572134	1.979954	-0.255200
14	2.382184	0.405754	-0.493534
8	3.437183	-0.803207	-0.584115
12	2.228182	-2.005772	0.322794
8	0.517567	-2.678364	-0.064824
12	-0.993596	-2.368421	1.128408
8	-2.394936	-1.858162	-0.155309
14	-2.394191	-0.271795	-0.486551
8	-3.203935	0.911555	0.217904
12	-1.715006	2.049967	0.758540
8	-0.530226	2.859707	-0.534653
12	-0.347642	1.397796	-1.776583
8	1.135140	0.127214	-1.582538
26	-0.247886	-1.245233	-1.145927
8	-1.724789	-0.000804	-1.982797

14	0.153937	0.095199	1.706776
8	-0.071619	1.702126	1.998263
8	-0.757682	0.028708	0.246450
8	-0.389150	-1.146128	2.547416
NCl-Fe16_T			
8	1.633489	-0.030283	1.100788
12	1.031007	2.775666	0.377622
8	2.569296	1.953801	-0.412631
14	2.361825	0.369205	-0.494090
8	3.381314	-0.874930	-0.475252
12	2.172534	-1.934158	0.602864
8	0.477560	-2.633419	0.111711
12	-1.037839	-2.127580	1.290445
8	-2.610061	-1.806047	0.190935
14	-2.383461	-0.339306	-0.422129
8	-3.197502	1.003867	-0.091688
12	-1.725449	2.097993	0.594325
8	-0.522814	2.811790	-0.744091
12	-0.405589	1.228222	-1.814717
8	1.111520	0.019003	-1.573191
26	-0.078475	-1.490347	-1.292625
8	-1.607841	-0.358669	-1.921030
14	0.130411	0.295818	1.749464
8	-0.043863	1.927578	1.910996
8	-0.863702	0.121192	0.384591
8	-0.314705	-0.920471	2.685910
NCl-Fe2_Q			
8	-1.125292	1.156419	0.968899
26	-2.105230	-1.529775	0.418951
8	-3.097917	-0.093007	-0.308689
14	-2.043287	1.096305	-0.587056
8	-2.201486	2.697554	-0.667763
12	-0.578229	3.017924	0.350013
8	1.208541	2.644113	-0.197652
12	2.307466	1.551721	1.011358
8	3.361768	0.306392	-0.049435
14	2.381378	-0.856141	-0.560013
8	2.331728	-2.382855	-0.064737
12	0.540479	-2.499247	0.681093
8	-0.904554	-2.549757	-0.627732
12	-0.178211	-1.203982	-1.794305
8	-0.924819	0.610415	-1.739069
12	0.943393	1.263128	-1.531359
8	1.718233	-0.542292	-2.074896
14	0.023121	0.124749	1.597680
8	-0.647779	-1.345678	1.923054
8	0.839553	-0.305902	0.166843
8	1.099552	0.943453	2.445817
NCl-Fe2_S			
8	-0.972545	1.315303	0.972665
26	-2.271675	-1.370371	0.384911
8	-2.961644	0.180216	-0.314849
14	-1.859334	1.334682	-0.579169
8	-1.910633	2.944944	-0.642764
12	-0.242387	3.104318	0.355571
8	1.506003	2.511213	-0.124916
12	2.429507	1.267794	1.090902
8	3.348902	-0.043258	-0.011099

14	2.271005	-1.101666	-0.553238
8	2.062727	-2.616691	-0.065276
12	0.251137	-2.548929	0.634924
8	-1.182026	-2.418617	-0.672779
12	-0.313239	-1.095519	-1.768631
8	-0.786826	0.800913	-1.747754
12	1.146712	1.192010	-1.506237
8	1.672554	-0.695735	-2.068426
14	-0.018803	0.097549	1.571961
8	-0.905988	-1.275610	1.814546
8	0.770243	-0.408343	0.151384
8	1.147064	0.701373	2.479295
NCl-Fe2_T			
8	-1.155343	1.097283	0.979654
26	-2.069937	-1.556259	0.411283
8	-3.067942	-0.170423	-0.376571
14	-2.055594	1.069328	-0.593716
8	-2.258813	2.666756	-0.610295
12	-0.635621	2.983911	0.413085
8	1.160749	2.666617	-0.142450
12	2.271515	1.562773	1.043189
8	3.348210	0.361531	-0.046652
14	2.389004	-0.808606	-0.581721
8	2.367142	-2.345229	-0.114035
12	0.592204	-2.508896	0.658987
8	-0.875611	-2.507041	-0.624183
12	-0.173972	-1.146106	-1.793661
8	-0.916618	0.661825	-1.751690
12	0.942264	1.321595	-1.521640
8	1.724038	-0.476271	-2.090031
14	0.014040	0.078496	1.592433
8	-0.610731	-1.417813	1.898781
8	0.838805	-0.296049	0.151282
8	1.070786	0.903110	2.459836
NCl-Fe6_Q			
8	1.397565	0.495085	0.998584
12	-0.306356	2.857229	0.683092
8	1.422662	2.884543	-0.135182
14	1.841805	1.379087	-0.487682
8	3.290960	0.651656	-0.604637
26	2.632762	-0.986244	0.101784
8	1.349160	-2.260971	-0.333735
12	-0.152399	-2.598976	0.899434
8	-1.756463	-2.736799	-0.200935
14	-2.211109	-1.246815	-0.592284
8	-3.453931	-0.416506	-0.011271
12	-2.550653	1.116771	0.766225
8	-1.792741	2.413297	-0.452598
12	-1.094193	1.181137	-1.738428
8	0.834174	0.764612	-1.686208
12	0.311631	-1.147048	-1.557438
8	-1.610843	-0.752265	-2.085181
14	-0.069933	0.048794	1.638427
8	-0.914576	1.411003	2.028222
8	-0.881119	-0.333692	0.187371
8	0.015294	-1.345205	2.408141
NCl-Fe6_S			
8	1.467676	0.394560	0.952415

12	-0.228020	2.856859	0.728299
8	1.505101	2.836821	-0.083668
14	1.840431	1.340838	-0.540177
8	3.216970	0.496124	-0.732703
26	2.531801	-0.987862	0.148216
8	1.309693	-2.224622	-0.414030
12	-0.174128	-2.615502	0.835932
8	-1.814126	-2.714070	-0.205262
14	-2.219600	-1.209062	-0.582688
8	-3.435079	-0.349180	0.018947
12	-2.479586	1.127938	0.841310
8	-1.756105	2.456561	-0.364160
12	-1.153420	1.236843	-1.711490
8	0.769465	0.842527	-1.720330
12	0.321253	-1.079925	-1.622197
8	-1.631404	-0.701413	-2.074431
14	-0.010937	-0.003039	1.633459
8	-0.782016	1.387612	2.059056
8	-0.871648	-0.322228	0.201200
8	0.046659	-1.406751	2.379944
NCl-Fe6_T			
8	1.447763	0.372130	0.968035
12	-0.183502	2.872435	0.709504
8	1.551372	2.819925	-0.083450
14	1.910028	1.316798	-0.496754
8	3.317120	0.520590	-0.605413
26	2.521194	-1.061045	0.097737
8	1.244263	-2.322572	-0.341782
12	-0.263105	-2.626285	0.882184
8	-1.877523	-2.663778	-0.207944
14	-2.253624	-1.154564	-0.601119
8	-3.456098	-0.267969	-0.016162
12	-2.479100	1.204959	0.785726
8	-1.688368	2.492337	-0.420537
12	-1.053759	1.240637	-1.724094
8	0.861666	0.771876	-1.691300
12	0.283907	-1.133488	-1.567364
8	-1.628414	-0.675670	-2.088869
14	-0.049181	0.016214	1.630106
8	-0.800668	1.425031	2.034521
8	-0.887353	-0.293215	0.181368
8	-0.046942	-1.379958	2.393549
NCl-Fe8_Q			
8	1.362343	-0.953594	0.961838
12	2.212056	1.849556	0.870744
8	3.344336	0.551176	0.041573
14	2.436689	-0.664526	-0.474359
8	2.728350	-2.235813	-0.687049
12	1.066116	-2.782178	0.151306
8	-0.674390	-2.509206	-0.569956
26	-1.988532	-1.582757	0.537787
8	-3.108383	-0.258109	-0.352231
14	-2.132243	0.975580	-0.691029
8	-2.224954	2.450394	-0.069827
12	-0.525778	2.581779	0.857570
8	1.021766	2.839259	-0.269906
12	0.509152	1.622888	-1.655936
8	1.386241	-0.138381	-1.675134

12	-0.417441	-0.947193	-1.702221
8	-1.308970	0.828901	-2.150676
14	0.078037	-0.098141	1.595054
8	0.628291	1.373327	2.105189
8	-0.641662	0.424965	0.136120
8	-0.985741	-1.088835	2.248141

NCl-Fe8_S

8	0.970686	-1.311357	0.974441
12	2.663507	1.151301	0.905629
8	3.305150	-0.436451	0.052859
14	2.099486	-1.360934	-0.459851
8	1.942161	-2.956851	-0.632798
12	0.170715	-2.970885	0.150147
8	-1.424273	-2.178165	-0.536020
26	-2.418437	-1.055632	0.590878
8	-2.822808	0.436279	-0.473884
14	-1.668552	1.552053	-0.714120
8	-1.486334	2.981794	-0.016022
12	0.264257	2.670558	0.834190
8	1.860328	2.464508	-0.250909
12	1.030924	1.373948	-1.617242
8	1.245177	-0.589914	-1.676687
12	-0.757637	-0.723808	-1.658797
8	-0.932646	1.263321	-2.189522
14	0.037412	-0.052952	1.526845
8	0.999457	1.142573	2.133643
8	-0.313588	0.730097	0.070893
8	-1.360643	-0.608489	2.085234

NCl-Fe8_T

8	1.361005	-0.989503	0.938460
12	2.249797	1.764672	0.911909
8	3.349597	0.476506	0.011402
14	2.413903	-0.716152	-0.513559
8	2.647300	-2.295444	-0.744042
12	0.972857	-2.787516	0.116896
8	-0.772891	-2.426246	-0.571367
26	-2.006513	-1.533524	0.561889
8	-3.032500	-0.273146	-0.513033
14	-2.101753	1.031253	-0.697778
8	-2.229660	2.459954	0.016097
12	-0.490296	2.545741	0.904363
8	1.079581	2.817279	-0.195498
12	0.587237	1.660942	-1.638881
8	1.362118	-0.145288	-1.688125
12	-0.488523	-0.867915	-1.695248
8	-1.245695	0.971632	-2.139553
14	0.090258	-0.136771	1.582720
8	0.658740	1.300702	2.154368
8	-0.630252	0.465769	0.164231
8	-0.976997	-1.164222	2.192440

NCs-Fe13_Q

8	1.969806	-1.841699	0.047256
14	0.363082	-1.745611	-0.156873
8	0.312893	-0.000555	-0.275806
8	-0.541111	-2.345813	-1.352031
8	-0.696347	1.851030	1.142168
12	-1.187183	0.004575	1.445670
14	0.376790	1.744464	-0.155627

8	-0.709726	-1.845551	1.142110
8	1.984064	1.827586	0.049292
12	-2.117581	1.733372	-0.441432
8	-2.717780	0.009220	0.131313
8	-0.521872	2.351117	-1.351744
26	2.394015	-0.008745	0.050761
12	-2.132070	-1.721219	-0.438008
NCs-Fe13_S			
8	1.990311	-1.790892	0.301504
14	0.419804	-1.685789	-0.107029
8	0.516843	0.000066	-0.588097
8	-0.424328	-2.414645	-1.280701
8	-0.735024	1.673655	1.117640
12	-1.499653	-0.000373	1.551238
14	0.418773	1.685860	-0.107100
8	-0.734099	-1.673982	1.117654
8	1.989251	1.791957	0.301357
12	-2.057294	1.702440	-0.541137
8	-2.770250	-0.000707	-0.000803
8	-0.425764	2.414186	-1.280818
26	2.321611	0.000633	-0.004976
12	-2.056176	-1.703282	-0.541326
NCs-Fe13_T			
8	1.988469	-1.824229	0.119871
14	0.396131	-1.703522	-0.171973
8	0.414280	0.000120	-0.525787
8	-0.506431	-2.396828	-1.320552
8	-0.689368	1.731673	1.122688
12	-1.354054	-0.000860	1.540491
14	0.393873	1.703691	-0.172205
8	-0.687259	-1.732540	1.122704
8	1.986084	1.826572	0.119535
12	-2.099690	1.707787	-0.469139
8	-2.757808	-0.001530	0.107027
8	-0.509687	2.395903	-1.320654
26	2.370981	0.001436	0.084646
12	-2.097240	-1.709662	-0.469764
NCs-Fe14_Q			
8	-2.898800	-0.832606	0.023563
14	-1.901151	0.421335	0.227017
8	-0.352744	-0.415282	-0.422578
8	-1.806799	1.652778	-0.847254
8	1.610245	-0.863448	1.281953
12	0.502168	0.701487	1.659009
14	0.983158	-1.536371	-0.139638
8	-1.392036	0.814737	1.712417
8	0.135361	-2.909314	-0.135046
12	2.712058	0.274810	-0.024825
8	1.553923	1.770741	0.270546
8	2.145996	-1.133424	-1.199398
12	-1.591490	-2.143755	-0.366904
26	0.054535	1.728713	-0.842473
NCs-Fe14_S			
8	-0.529383	2.848922	0.182930
14	0.451774	1.599413	-0.121055
8	-0.752265	0.458336	-0.541367
8	1.651829	1.428974	-1.215996
8	-1.033208	-1.547953	1.132221

12	0.673046	-0.879606	1.606505
14	-1.899539	-0.784702	-0.090468
8	1.292687	0.876704	1.166030
8	-3.132673	0.204133	0.260562
12	-0.012720	-2.332675	-0.626323
8	1.658130	-1.713131	0.087866
8	-1.766468	-1.879924	-1.279827
12	-2.165070	1.845395	0.005338
26	2.277556	-0.015839	-0.277087
Ncs-Fe14_T			
8	-0.855133	2.801991	0.341015
14	0.285315	1.729220	-0.056931
8	-0.753796	0.455867	-0.580875
8	1.503639	1.813276	-1.132820
8	-0.842589	-1.624983	1.107758
12	0.809062	-0.865878	1.650028
14	-1.714902	-0.941959	-0.165106
8	1.172148	0.944911	1.166069
8	-3.086689	-0.145246	0.169541
12	0.269478	-2.461465	-0.505669
8	1.863894	-1.634569	0.169046
8	-1.415066	-2.032548	-1.329197
12	-2.340753	1.614673	0.032983
26	2.094981	0.188492	-0.396303
NCs-Fe6_Q			
8	-2.298900	1.868682	0.309583
14	-0.772994	1.689960	-0.200951
8	-0.870439	0.002625	-0.592790
8	0.000384	2.398706	-1.436728
8	0.471584	-1.705711	0.952854
26	1.220182	-0.003952	1.274458
14	-0.783848	-1.685342	-0.200805
8	0.482386	1.702576	0.952949
8	-2.310832	-1.854177	0.309834
12	1.664842	-1.697307	-0.808158
8	2.445442	-0.007544	-0.340824
8	-0.015145	-2.398895	-1.436733
12	-2.771303	0.008747	0.177573
12	1.676060	1.687560	-0.807455
NCs-Fe16_S			
8	-2.301380	1.848577	0.399852
14	-0.811691	1.645160	-0.200137
8	-0.974708	0.000857	-0.690513
8	-0.057854	2.424022	-1.406546
8	0.480133	-1.561450	0.910249
26	1.384980	-0.001448	1.239504
14	-0.815124	-1.643805	-0.200027
8	0.483277	1.560418	0.910331
8	-2.305203	-1.844053	0.400024
12	1.619124	-1.684024	-0.826188
8	2.441221	-0.002287	-0.364969
8	-0.062945	-2.424123	-1.406524
12	-2.813238	0.002794	0.265170
12	1.622914	1.681479	-0.825653
NCs-Fe6_T			
8	1.862074	2.305907	0.258683
14	1.718315	0.762449	-0.206849
8	-0.004021	0.784339	-0.473221

8	2.376616	0.002106	-1.475186
8	-1.783675	-0.512436	0.946411
26	0.005556	-1.122103	1.229928
14	-1.726093	0.745406	-0.206694
8	1.788635	-0.494609	0.946494
8	-1.885051	2.287327	0.258945
12	-1.718178	-1.694011	-0.755740
8	0.012007	-2.377144	-0.255029
8	-2.376730	-0.021283	-1.475175
12	-0.013619	2.727097	0.173967
12	1.735597	-1.677166	-0.755219

H2_NCl-Fe12_Q

8	-1.615857	-0.626643	1.070073
12	0.385223	-2.673475	0.476669
8	-1.380963	-2.939245	-0.205068
14	-2.069525	-1.509245	-0.447142
8	-3.594372	-0.985947	-0.404754
12	-3.124402	0.634136	0.565633
8	-2.110566	2.116200	-0.080126
12	-0.549302	2.640087	1.001613
8	0.956930	3.095831	-0.159513
14	1.511663	1.693914	-0.702696
8	2.911547	0.999382	-0.293509
26	2.575213	-0.755495	0.379348
8	1.697160	-1.995111	-0.775205
12	0.689876	-0.769208	-1.866084
8	-1.262386	-0.700218	-1.680414
12	-1.062994	1.267904	-1.481503
8	0.877613	1.222775	-2.187173
14	-0.145402	-0.007293	1.574904
8	0.900684	-1.249253	1.798345
8	0.373778	0.590012	0.070845
8	-0.365078	1.310038	2.451298
1	3.634746	-1.278819	1.801059
1	4.086664	-1.457465	1.190677

H2_NCl-Fe12_S

8	-1.651298	-0.454761	1.018682
12	0.096516	-2.789680	0.411202
8	-1.686160	-2.752117	-0.316627
14	-2.191506	-1.246078	-0.513997
8	-3.646126	-0.543351	-0.467098
12	-2.990601	0.969841	0.556773
8	-1.773305	2.316069	-0.044827
12	-0.209406	2.621989	1.101929
8	1.338844	2.908532	-0.026707
14	1.756572	1.513617	-0.685124
8	3.089869	0.636732	-0.449333
26	2.235216	-0.852647	0.449493
8	1.457020	-2.136749	-0.765963
12	0.645611	-0.795629	-1.843494
8	-1.287641	-0.471314	-1.700279
12	-0.941948	1.466243	-1.567427
8	0.958980	1.198582	-2.121376
14	-0.138362	-0.119441	1.625639
8	0.670461	-1.523157	1.849322
8	0.698541	0.345851	0.192580
8	-0.213910	1.224812	2.484337
1	3.635145	-1.697014	0.227160

1	3.431122	-1.873751	0.985311

H2_NCl-Fe12_T

8	-1.621763	-0.582560	1.086129
12	0.230859	-2.704259	0.400485
8	-1.557146	-2.874616	-0.244499
14	-2.152609	-1.396366	-0.450868
8	-3.636120	-0.769211	-0.370490
12	-3.056838	0.788647	0.645517
8	-1.983044	2.227693	-0.004833
12	-0.333052	2.614344	1.022252
8	1.219099	3.020011	-0.113269
14	1.589940	1.597341	-0.752525
8	2.917527	0.715932	-0.497832
26	2.505136	-0.927944	0.443650
8	1.591694	-1.995825	-0.797213
12	0.649346	-0.731961	-1.898718
8	-1.308444	-0.625101	-1.678278
12	-1.057000	1.336733	-1.462576
8	0.836467	1.251491	-2.215503
14	-0.117269	-0.032318	1.560557
8	0.869268	-1.341657	1.740236
8	0.371412	0.604532	0.065719
8	-0.238991	1.264910	2.481982
1	3.528528	-0.675083	1.959148
1	3.977610	-0.366416	1.404913

H2_NCl-Fe14_Q

8	-1.775543	0.374240	0.944129
12	-0.779016	-2.332952	1.332774
8	-2.387694	-2.135265	0.328908
14	-2.323485	-0.712797	-0.410519
8	-3.459655	0.320887	-0.900491
12	-2.508659	1.872257	-0.224301
8	-0.862635	2.574076	-0.873384
12	0.586386	2.835073	0.429072
8	2.288878	2.344291	-0.389514
14	2.311550	0.741380	-0.441722
8	3.229185	-0.251732	0.426071
12	1.846521	-1.227680	1.372936
8	0.878172	-2.591244	0.374559
26	0.752642	-1.631911	-1.240588
8	-1.056444	-0.688657	-1.501818
12	-0.089140	1.006852	-1.720307
8	1.701646	0.102090	-1.872258
14	-0.300566	0.572283	1.687412
8	0.094657	-0.844263	2.442878
8	0.743841	0.403454	0.355157
8	-0.088088	2.086487	2.144465
1	0.457369	-2.727062	-2.763785
1	1.225296	-2.652920	-2.785028

H2_NCl-Fe14_S

8	-1.713866	0.286550	1.046287
12	-0.848153	-2.552401	0.964972
8	-2.458492	-2.060164	0.059126
14	-2.350259	-0.544093	-0.438842
8	-3.449582	0.600669	-0.728924
12	-2.396929	1.971964	0.146896
8	-0.754137	2.714208	-0.473226
12	0.729166	2.730785	0.802644

8	2.382441	2.218294	-0.032343
14	2.313120	0.680285	-0.465337
8	3.212597	-0.510273	0.137194
12	1.874976	-1.595403	1.085302
8	0.760900	-2.729485	-0.041883
26	0.596178	-1.244413	-1.250502
8	-1.115082	-0.345649	-1.554973
12	-0.142255	1.346840	-1.713120
8	1.591544	0.455799	-1.961384
14	-0.193260	0.231221	1.713270
8	0.129217	-1.276088	2.280105
8	0.768861	0.090620	0.288414
8	0.182110	1.646916	2.339124
1	0.653889	-1.927812	-2.766365
1	0.177325	-2.413837	-2.348324

H2_NCl-Fe14_T

8	-1.850422	0.304229	0.868370
12	-0.800323	-2.385784	1.268412
8	-2.399760	-2.219861	0.241534
14	-2.267843	-0.808188	-0.499608
8	-3.348450	0.206149	-1.131528
12	-2.562626	1.787859	-0.324669
8	-0.917079	2.548517	-0.890827
12	0.470700	2.818631	0.486971
8	2.247335	2.436307	-0.257566
14	2.284957	0.836864	-0.351404
8	3.182562	-0.190612	0.499225
12	1.770857	-1.182923	1.389615
8	0.874606	-2.572833	0.351493
26	0.906824	-1.568434	-1.246924
8	-0.884807	-0.778807	-1.455481
12	-0.083204	1.004505	-1.711355
8	1.736253	0.221663	-1.821228
14	-0.421340	0.555423	1.690112
8	-0.010648	-0.868571	2.420295
8	0.707191	0.494600	0.419045
8	-0.312098	2.072302	2.174683
1	2.344016	-2.242764	-2.117673
1	1.995400	-2.887437	-1.861520

H2_NCl-Fe16_Q

8	1.606014	-0.004346	1.150197
12	1.237542	2.741252	0.180241
8	2.765245	1.770464	-0.444627
14	2.411751	0.206936	-0.466471
8	3.305569	-1.126705	-0.293411
12	1.995034	-1.961249	0.860628
8	0.252983	-2.600302	0.398023
12	-1.232374	-1.892320	1.494166
8	-2.773693	-1.541153	0.369673
14	-2.413513	-0.174522	-0.391416
8	-3.108345	1.259396	-0.191129
12	-1.573661	2.308016	0.401762
8	-0.298655	2.787525	-0.970136
12	-0.299206	1.089481	-1.859818
8	1.200599	-0.115264	-1.572898
26	-0.161495	-1.650001	-1.200928
8	-1.647255	-0.412992	-1.872484
14	0.119809	0.469024	1.730434

8	0.047812	2.115198	1.749909
8	-0.843321	0.218890	0.351947
8	-0.424963	-0.616214	2.770221
1	-0.174638	-2.853861	-2.732575
1	0.536913	-2.564382	-2.744972

H2_NCl-Fe16_S

8	1.660970	-0.110299	1.146392
12	1.098934	2.714155	0.468006
8	2.665485	1.920366	-0.272514
14	2.394999	0.349819	-0.451211
8	3.376488	-0.922376	-0.494788
12	2.144816	-2.011816	0.525288
8	0.421260	-2.645758	0.129171
12	-1.120703	-2.180974	1.244397
8	-2.614204	-1.766896	0.022846
14	-2.394956	-0.240949	-0.441425
8	-3.132095	1.057744	0.137303
12	-1.670923	2.187938	0.671912
8	-0.449073	2.859407	-0.659644
12	-0.340020	1.350713	-1.839016
8	1.141075	0.120065	-1.543945
26	-0.184643	-1.305791	-1.182515
8	-1.688150	-0.082164	-1.950015
14	0.134790	0.180148	1.737424
8	-0.068031	1.808405	1.904788
8	-0.755309	-0.061452	0.287303
8	-0.420815	-0.984606	2.671620
1	-0.064314	-2.014457	-2.687782
1	0.531317	-2.340927	-2.269001

H2_NCl-Fe16_T

8	1.667279	0.034358	1.099005
12	1.225209	2.778489	0.081761
8	2.655042	1.753084	-0.677517
14	2.373068	0.184050	-0.540033
8	3.335754	-1.095766	-0.387231
12	2.070782	-1.946411	0.807561
8	0.336956	-2.587045	0.405053
12	-1.097492	-1.848251	1.536711
8	-2.687352	-1.553955	0.463631
14	-2.394383	-0.177065	-0.307397
8	-3.128422	1.240469	-0.129353
12	-1.574236	2.312376	0.419686
8	-0.351266	2.786268	-1.006341
12	-0.347448	1.057953	-1.838401
8	1.070427	-0.254649	-1.522957
26	-0.214076	-1.702439	-1.230746
8	-1.676087	-0.427567	-1.813695
14	0.203538	0.535262	1.729695
8	0.152475	2.183489	1.725521
8	-0.849135	0.309167	0.419648
8	-0.287558	-0.550967	2.795087
1	-1.367338	-2.917420	-1.888117
1	-0.844475	-3.355571	-1.518814

H2_NCl-Fe2_Q

8	-0.749661	1.412510	0.956300
26	-2.548266	-0.925589	0.278038
8	-2.925877	0.789516	-0.427810
14	-1.577713	1.651631	-0.620337

8	-1.285521	3.236151	-0.651276
12	0.327144	3.057019	0.421269
8	1.957526	2.225365	-0.110978
12	2.663142	0.846446	1.097099
8	3.356780	-0.632478	0.041881
14	2.106658	-1.457864	-0.532535
8	1.606413	-2.917263	-0.086935
12	-0.163869	-2.520414	0.626241
8	-1.517178	-2.146686	-0.728338
12	-0.391651	-1.045291	-1.831139
8	-0.603670	0.903006	-1.761702
12	1.362955	1.002575	-1.491060
8	1.620971	-0.938580	-2.058653
14	0.048648	0.091967	1.592878
8	-0.982911	-1.145211	1.890421
8	0.752424	-0.510877	0.158434
8	1.286614	0.589125	2.474656
1	-4.008962	-1.590997	1.314159
1	-3.522329	-1.344595	1.859852
H2_NCl-Fe2_S			
8	-0.510721	1.564914	0.979988
26	-2.626084	-0.776193	0.381672
8	-2.773128	0.987714	-0.231610
14	-1.408883	1.788099	-0.542338
8	-1.032466	3.353990	-0.651705
12	0.641117	3.090693	0.314453
8	2.162361	2.046549	-0.170688
12	2.731912	0.610500	1.054132
8	3.280796	-0.906778	-0.032163
14	1.955258	-1.645479	-0.552947
8	1.359608	-3.044991	-0.038903
12	-0.358909	-2.493668	0.683494
8	-1.718222	-2.057026	-0.626234
12	-0.552104	-0.991509	-1.732396
8	-0.545266	0.965008	-1.722539
12	1.433498	0.851970	-1.520244
8	1.462658	-1.114478	-2.069214
14	0.073437	0.135020	1.575708
8	-1.155838	-0.938563	1.792836
8	0.698815	-0.567775	0.150153
8	1.369897	0.399078	2.469775
1	-4.181537	-1.053638	-0.190058
1	-3.751744	-0.969274	-0.850156
H2_NCl-Fe2_T			
8	-0.985585	1.219809	0.939246
26	-2.341148	-1.204748	0.370867
8	-2.966830	0.318637	-0.626575
14	-1.774756	1.396888	-0.698869
8	-1.734068	3.006642	-0.629525
12	-0.133819	3.013815	0.477729
8	1.626423	2.450826	-0.001316
12	2.477175	1.134360	1.182332
8	3.406147	-0.189441	0.088973
14	2.291385	-1.166090	-0.530638
8	1.985243	-2.695110	-0.142893
12	0.168807	-2.546287	0.534496
8	-1.236940	-2.184616	-0.774000
12	-0.235240	-1.015165	-1.907251

8	-0.625557	0.891652	-1.805697
12	1.288706	1.211993	-1.450436
8	1.766521	-0.676209	-2.049822
14	-0.007625	0.033346	1.585545
8	-0.857408	-1.360909	1.842102
8	0.829101	-0.425262	0.179038
8	1.111072	0.675348	2.527897
1	-3.607232	-1.318457	1.738059
1	-3.981478	-0.891662	1.212999

H2_NCl-Fe6_Q

8	-0.510721	1.564914	0.979988
26	-2.626084	-0.776193	0.381672
8	-2.773128	0.987714	-0.231610
14	-1.408883	1.788099	-0.542338
8	-1.032466	3.353990	-0.651705
12	0.641117	3.090693	0.314453
8	2.162361	2.046549	-0.170688
12	2.731912	0.610500	1.054132
8	3.280796	-0.906778	-0.032163
14	1.955258	-1.645479	-0.552947
8	1.359608	-3.044991	-0.038903
12	-0.358909	-2.493668	0.683494
8	-1.718222	-2.057026	-0.626234
12	-0.552104	-0.991509	-1.732396
8	-0.545266	0.965008	-1.722539
12	1.433498	0.851970	-1.520244
8	1.462658	-1.114478	-2.069214
14	0.073437	0.135020	1.575708
8	-1.155838	-0.938563	1.792836
8	0.698815	-0.567775	0.150153
8	1.369897	0.399078	2.469775
1	-4.181537	-1.053638	-0.190058
1	-3.751744	-0.969274	-0.850156

H2_NCl-Fe6_S

8	1.362426	0.505965	0.930679
12	-0.590454	2.844214	0.710532
8	1.152414	2.976419	-0.060318
14	1.651851	1.524446	-0.506470
8	3.139011	0.880810	-0.677964
26	2.701180	-0.714364	0.158060
8	1.483205	-2.032939	-0.335056
12	0.042082	-2.595139	0.878069
8	-1.555497	-2.865625	-0.202766
14	-2.133545	-1.420880	-0.595825
8	-3.445071	-0.696406	-0.017809
12	-2.639985	0.879747	0.798849
8	-2.047066	2.276795	-0.405500
12	-1.289240	1.111478	-1.724588
8	0.669452	0.906383	-1.707616
12	0.389071	-1.048106	-1.580238
8	-1.578136	-0.865672	-2.084625
14	-0.081041	0.020705	1.628249
8	-0.978776	1.339227	2.038027
8	-0.915152	-0.375076	0.197515
8	0.077612	-1.356041	2.407854
1	3.710476	-1.467036	-0.913823
1	4.084088	-1.556341	-0.209938

H2_NCl-Fe6_T

8	1.378519	0.453494	0.919838
12	-0.501052	2.862818	0.720245
8	1.233299	2.950571	-0.060069
14	1.734084	1.497490	-0.500679
8	3.224210	0.870267	-0.618414
26	2.656094	-0.783745	0.121010
8	1.395817	-2.147940	-0.326655
12	-0.055857	-2.637337	0.874978
8	-1.669734	-2.806651	-0.207920
14	-2.195592	-1.343338	-0.601622
8	-3.476734	-0.576118	-0.013106
12	-2.612722	0.971498	0.791066
8	-1.963619	2.344587	-0.408584
12	-1.213903	1.153503	-1.712785
8	0.741381	0.861057	-1.694179
12	0.330675	-1.088457	-1.553930
8	-1.615965	-0.805790	-2.088440
14	-0.085801	0.009909	1.613904
8	-0.932115	1.358354	2.035843
8	-0.930238	-0.337734	0.180052
8	0.023914	-1.374681	2.387076
1	3.773902	-1.866151	-0.577890
1	4.194383	-1.512947	-0.009227

H2_NCl-Fe8_Q

8	0.954287	-1.355187	0.956890
12	2.725266	0.983326	0.995776
8	3.365932	-0.611601	0.150090
14	2.121202	-1.439487	-0.429429
8	1.857341	-3.013552	-0.668773
12	0.069665	-2.940876	0.086085
8	-1.445659	-2.060610	-0.664965
26	-2.543616	-0.884937	0.438332
8	-2.868657	0.752658	-0.530163
14	-1.556004	1.665260	-0.744961
8	-1.236921	3.074572	-0.049946
12	0.409464	2.617982	0.899188
8	2.015117	2.356402	-0.152680
12	1.176880	1.386166	-1.581467
8	1.369048	-0.574453	-1.656498
12	-0.609535	-0.669253	-1.739619
8	-0.777223	1.315533	-2.192089
14	0.020783	-0.107137	1.550013
8	1.024208	1.057685	2.160600
8	-0.332313	0.686868	0.087571
8	-1.356960	-0.667268	2.113302
1	-3.761758	-1.276205	1.806820
1	-4.114410	-1.592842	1.191565

H2_NCl-Fe8_S

8	0.869582	1.409699	-0.978460
12	2.833894	-0.773105	-0.917230
8	3.302534	0.881907	-0.074384
14	1.980054	1.619907	0.452812
8	1.585828	3.174275	0.632983
12	-0.163926	2.939430	-0.172705
8	-1.630526	1.943793	0.525397
26	-2.644910	0.721507	-0.564523
8	-2.748225	-0.934872	0.377999
14	-1.409788	-1.780282	0.694941

8	-0.975788	-3.176324	0.034773
12	0.678667	-2.617674	-0.847732
8	2.226756	-2.189594	0.236838
12	1.242408	-1.251703	1.611409
8	1.256063	0.726664	1.673205
12	-0.736590	0.621634	1.641845
8	-0.744407	-1.361538	2.180238
14	0.062226	0.058835	-1.513226
8	1.160212	-1.008035	-2.134610
8	-0.178267	-0.753685	-0.053649
8	-1.405181	0.456107	-2.011027
1	-3.853725	1.076982	0.699700
1	-4.235606	1.215258	0.033054
H2_NCl-Fe8_T			
8	1.007181	-1.345942	0.946107
12	2.670636	1.037678	1.039487
8	3.350726	-0.482682	0.085370
14	2.136306	-1.371708	-0.474194
8	1.942701	-2.957052	-0.708847
12	0.158439	-2.938583	0.055674
8	-1.398878	-2.063134	-0.622111
26	-2.481560	-0.995023	0.493819
8	-2.732720	0.498868	-0.813488
14	-1.571998	1.628345	-0.780149
8	-1.433952	2.991082	0.049160
12	0.286693	2.588714	0.936644
8	1.930669	2.417511	-0.080999
12	1.209826	1.425471	-1.563579
8	1.313383	-0.539781	-1.670681
12	-0.703385	-0.594579	-1.723132
8	-0.691145	1.439691	-2.185446
14	0.024552	-0.145853	1.543989
8	0.969113	1.033983	2.208432
8	-0.344339	0.692399	0.116774
8	-1.332318	-0.792845	2.092601
1	-4.056711	-0.340633	1.099730
1	-3.776618	-0.700948	1.729829
H2_NCs-Fe6_Q			
8	1.918860	-1.838154	-0.031690
14	0.308143	-1.741788	-0.186323
8	0.243400	0.000044	-0.305421
8	-0.631942	-2.349345	-1.351440
8	-0.728397	1.846945	1.147262
12	-1.197829	-0.001808	1.462272
14	0.302843	1.741960	-0.186904
8	-0.723268	-1.849174	1.147288
8	1.913347	1.843266	-0.032544
12	-2.199544	1.722592	-0.388285
8	-2.775695	-0.003446	0.202275
8	-0.639383	2.347167	-1.351459
26	2.361808	0.003290	-0.016622
12	-2.193897	-1.726801	-0.390186
1	4.258733	0.379432	1.028766
1	4.260312	-0.373608	1.028791
H2_NCs-Fe6_S			
8	-1.938621	1.787119	0.262146
14	-0.359708	1.678124	-0.120757
8	-0.465988	0.000028	-0.579943

8	0.497593	2.404371	-1.286102
8	0.778028	-1.671913	1.118926
12	1.543654	0.000043	1.563867
14	-0.359970	-1.678089	-0.120566
8	0.778209	1.671956	1.118925
8	-1.938953	-1.786840	0.262140
12	2.121800	-1.700053	-0.524850
8	2.832607	-0.000231	0.026787
8	0.496988	-2.404687	-1.285946
26	-2.313293	0.000173	-0.039089
12	2.122167	1.699675	-0.524839
1	-3.936294	0.000500	0.191197
1	-3.612938	0.000110	0.938054
H2_NCs-Fe6_T			
8	-1.937550	1.890654	0.081809
14	-0.352576	1.739655	-0.175637
8	-0.474586	0.000289	-0.446599
8	0.583022	2.349557	-1.345113
8	0.736882	-1.747563	1.112723
12	1.368227	-0.001536	1.544839
14	-0.356680	-1.739576	-0.175281
8	0.740527	1.745788	1.112775
8	-1.941872	-1.886700	0.082343
12	2.156718	-1.710283	-0.451678
8	2.796279	-0.002593	0.133892
8	0.577484	-2.350912	-1.345168
26	-2.277117	0.002433	0.039057
12	2.160868	1.707094	-0.450570
1	-3.868044	0.399886	0.548160
1	-3.868593	-0.395720	0.544839
H2_NCs-Fe14_Q			
8	2.935224	0.767444	-0.021231
14	1.887507	-0.430289	0.267843
8	0.367809	0.421350	-0.393352
8	1.736902	-1.719272	-0.722850
8	-1.565702	1.091788	1.254048
12	-0.498363	-0.486640	1.710109
14	-0.916488	1.619883	-0.217241
8	1.384969	-0.717083	1.780639
8	-0.014083	2.953919	-0.326183
12	-2.712310	-0.104102	0.044435
8	-1.604182	-1.611624	0.432078
8	-2.097032	1.181536	-1.243647
12	1.680138	2.104040	-0.481157
26	-0.139738	-1.790655	-0.739947
1	-0.237849	-3.730246	-1.080330
1	-0.508068	-3.471096	-1.746135
H2_NCs-Fe14_S			
8	-0.656168	2.838847	0.207792
14	0.370189	1.618926	-0.065440
8	-0.784753	0.451508	-0.553421
8	1.613521	1.510508	-1.123442
8	-1.093425	-1.558874	1.127885
12	0.575615	-0.847772	1.675147
14	-1.912385	-0.823221	-0.145423
8	1.183969	0.890880	1.218798
8	-3.189451	0.130102	0.143710
12	0.023362	-2.352685	-0.552492

8 1.638625 -1.648843 0.214016
8 -1.693379 -1.927424 -1.314314
12 -2.255997 1.797279 -0.060904
26 2.275355 0.045293 -0.236779
1 2.730850 -0.554551 -1.690790
1 3.433397 -0.418417 -1.310076
H2_NCs-Fe14_T
8 -0.808751 2.826606 0.322037
14 0.306060 1.707665 -0.020448
8 -0.763167 0.471789 -0.574037
8 1.557106 1.745881 -1.061312
8 -1.015291 -1.590759 1.111053
12 0.637332 -0.859085 1.690498
14 -1.802551 -0.882166 -0.202792
8 1.139624 0.909283 1.216282
8 -3.153672 -0.026559 0.063805
12 0.135548 -2.475617 -0.450661
8 1.720552 -1.666444 0.266440
8 -1.495807 -1.990494 -1.348380
12 -2.327270 1.699420 -0.043742
26 2.152691 0.125358 -0.310283
1 3.421292 -0.220190 -1.351131
1 2.767540 -0.407123 -1.776411
H2_NCs-Fe6_Q
8 2.308656 -1.860177 0.441276
14 0.830560 -1.680891 -0.195236
8 0.961350 -0.002135 -0.605667
8 0.150179 -2.413045 -1.467317
8 -0.501988 1.656034 0.855080
26 -1.311994 0.003374 1.268235
14 0.839135 1.677472 -0.195169
8 -0.510125 -1.653344 0.855613
8 2.318044 1.849065 0.441490
12 -1.551755 1.662176 -0.988065
8 -2.397519 0.005416 -0.617358
8 0.162686 2.412606 -1.467627
12 2.799025 -0.006806 0.324931
12 -1.561119 -1.656463 -0.986613
1 -2.948569 0.009117 2.087609
1 -2.479385 0.008788 2.717007
H2_NCs-Fe6_S
8 -2.286175 1.843032 0.433193
14 -0.819329 1.648749 -0.226931
8 -0.993390 -0.000503 -0.701129
8 -0.123810 2.428750 -1.466604
8 0.527932 -1.583076 0.819589
26 1.395575 0.000769 1.247564
14 -0.817484 -1.649619 -0.227084
8 0.526365 1.583794 0.819353
8 -2.284139 -1.845621 0.432885
12 1.581848 -1.684567 -0.933977
8 2.356441 0.001241 -0.458939
8 -0.120773 -2.428749 -1.466574
12 -2.801214 -0.001543 0.299606
12 1.579613 1.686019 -0.934506
1 1.110946 0.001089 2.889113
1 0.376903 0.001231 2.562748
H2_NCs-Fe6_T

8	1.885705	2.275481	0.174123
14	1.742550	0.721842	-0.260191
8	0.000242	0.734730	-0.402756
8	2.337044	-0.040717	-1.554175
8	-1.839646	-0.543806	0.878798
26	-0.000323	-0.979482	1.239094
14	-1.742060	0.722850	-0.260230
8	1.839309	-0.544848	0.878866
8	-1.884331	2.276562	0.174117
12	-1.729307	-1.719324	-0.777612
8	-0.000694	-2.311858	-0.224009
8	-2.336971	-0.039335	-1.554242
12	0.000806	2.693739	0.126368
12	1.728247	-1.720306	-0.777575
1	-0.001064	-0.473933	2.831118
1	0.000372	0.215774	2.418402