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# Reactivity of Metal Catalysts in Glucose–Fructose Conversion

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## Comparison with other computational methods

For comparison the glucose to fructose isomerization with the $[AlO^1O^2(H_2O)_4]^{3+}$ catalyst was calculated at the B3LYP/6-31+G(d,p), the M06/6-31+G(d,p) and the PBE0/6-311+G(d,p) level. The energy trends are comparable to the PBE0/6-31+G(d,p) level used in this study (Table 18, Table 1). The only exception is the final fructofuranose-catalyst complex, which is less stabilized with the other functionals.

**Table 1: Relative free energies of different functionals for the isomerization with $[AlO^1O^2(H_2O)_4]^{3+}$ catalyst comparison with used method. Energy reference is glucosepyranose + $[Al(H_2O)_6]^{3+}$.**

| | ΔG(B3LYP/6-31+G**, CPCM(water)) / kcal $mol^{-1}$ | ΔG(M06/6-31+G**, CPCM(water)) / kcal $mol^{-1}$ | ΔG(PBE0/6-311+G**, CPCM(water)) / kcal $mol^{-1}$ | ΔG(PBE0/6-31+G**, CPCM(water)) / kcal $mol^{-1}$ |
|---|---|---|---|---|
| glucosepyranose + $[Al(H_2O)_6]^{3+}$ | 0.0 | 0.0 | 0.0 | 0.0 |
| glucopyranose | 6.4 | 3.0 | 0.8 | 2.3 |
| PT1 | | | | |
| glucopyranose O5 prot. | 11.0 | 10.8 | 6.9 | 11.0 |
| TS1 | | | | |
| glucose | 5.1 | 8.0 | 4.7 | 7.0 |
| DP2 | | | | |
| deprot. glucose | 12.0 | 10.1 | 9.2 | 10.4 |
| TS2 | 27.1 | 26.2 | 21.1 | 23.0 |
| deprot. fructose | 9.0 | 8.8 | 5.1 | 6.4 |
| RP2 | | | | |
| fructose | -1.7 | -2.4 | -3.0 | -1.3 |
| TS3 | 5.8 | 6.2 | 4.9 | 7.0 |
| fructofuranose O5 prot. | 6.0 | 4.4 | -0.1 | 0.7 |
| PT3 | | | | |
| fructofuranose | 0.1 | -1.4 | -5.1 | -13.9 |
| fructofuranose +$[Al(H_2O)_6]^{3+}$ | 2.7 | 2.8 | 1.5 | 1.5 |

## Influence of temperature and pressure

The computations reported in this study include thermal corrections for standard conditions (298 K and 1 bar). The experiments were carried out around 413 K and 80 bar. Therefore additional frequency calculations have been performed for exemplary aluminum(III) and iron(III) catalysts (Table 2, Table 19). Higher temperature will increase the importance of the entropic contributions, and higher pressure will favor more compact transition states. Nevertheless, only marginal to small differences are found (0.1 to 5.0 kcal/mol) for the relative TS2 barriers. Since temperature and pressure are not included in the optimization of the structures, the computed energy changes do not reflect all the effects of the experimental conditions.

**Table 2: Relative free energies at 298 K and 1 bar and at 413 K and 70 bar for critical steps (TS2 and product catalyst separation) in the glucose-fructose isomerization with selected $Al^{3+}$ and $Fe^{3+}$ catalysts (PBE0/6-31+G**, CPCM(water)).**

| | | ΔG(TS2) / kcal $mol^{-1}$ | ΔΔG(TS2) / kcal $mol^{-1}$ | ΔΔG(separation) / kcal $mol^{-1}$ |
|---|---|---|---|---|
| reference→ | | glucopyranose + $[M(H_2O)_6]^{3+}$ | lowest minimum before TS2 | glucopyranose-catalyst complex |
| catalyst ↓ | | | | |
| $[Al(H_2O)_6]^{3+}$ | 298 K, 1 bar | 24.4 | 29.2 | 9.4 |
| | 413 K, 70 bar | 25.2 | 28.7 | -- |
| $[AlO^1O^2(H_2O)_4]^{3+}$ | 298 K, 1 bar | 23.0 | 23.0 | 15.4 |
| | 413 K, 70 bar | 23.5 | 23.5 | -- |
| $[AlO^1O^2(H_2O)_3Cl]^{2+}$ | 298 K, 1 bar | 5.7 | 23.1 | 13.0 |
| | 413 K, 70 bar | 0.9 | 23.4 | 11.2 |
| $[Fe(H_2O)_6]^{3+}$ | 298 K, 1 bar | 21.0 | 25.4 | 13.0 |
| | 413 K, 70 bar | 27.4 | 30.4 | -- |
| $[FeO^1O^2(H_2O)_4]^{3+}$ | 298 K, 1 bar | 20.3 | 20.3 | 17.2 |
| | 413 K, 70 bar | 21.3 | 21.3 | -- |
| $[FeO^1O^2(H_2O)_3Cl]^{2+}$ | 298 K, 1 bar | -5.4 | 30.2 | 16.0 |
| | 413 K, 70 bar | -6.0 | 30.1 | 14.1 |

## Thermodynamic cyles

All mechanisms feature protonation and deprotonation reactions at hydroxyl groups and at the pyranic oxygen O5 (proton transfer 1 (PT1) from O1 to O5, proton transfer 2 (PT2) from O2 to O1, and proton transfer 3 (PT3) from O5 to O2, Figure 1). For the transition states of these transfers, we considered (a) direct proton transfer (intramolecular, concerted) and (b) proton transfers assisted by one to three water molecules (intermolecular, two steps). Mechanism (a) always led to the highest barriers. In the transition state for this intramolecular proton transfer, the O-H-O angle is very strained (for example, in the uncatalyzed reaction, PT1: γ(C1-H-O5) = 120°) whereas this angle is nearly linear in unconstrained proton transfers. Additionally, the chair conformation of the glucopyranose is distorted towards a boat conformation, thus raising the energy. In mechanism (b), the energy of the transition state is lowered the more waters are attached. The associated barriers depend on the number and position of the water molecules.

Free energies of proton transfer were calculated with the use of appropriate thermodynamic cycles (see below). The corresponding values in the Results section were always determined from such cycles. This approach was also used in a previous study on glucose protonation pathways.[1]

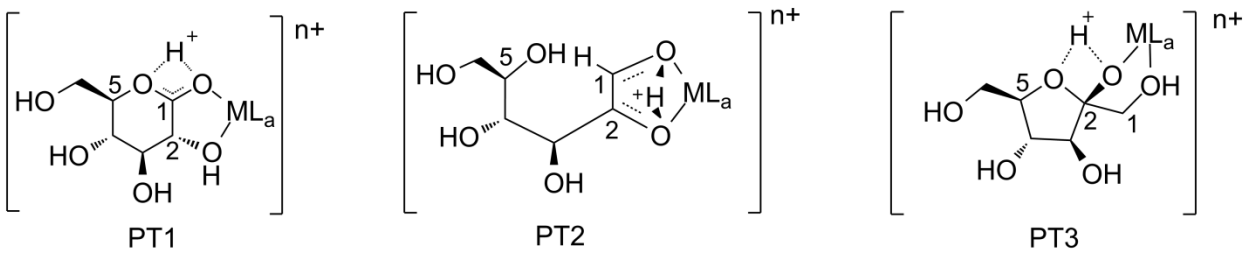
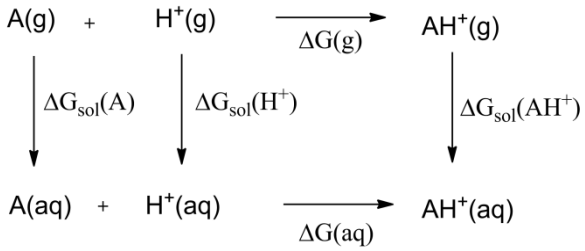



**Figure 1: The three proton transfers in the proposed glucose to fructose isomerization mechanism. PT1 from O1 to O5, PT2 from O2 to O1, and PT3 from O5 to O2.**

For the thermodynamic cycles the protonation reaction (1) was used or in case of deprotonations the back reaction of (1).

$$A + H^+ \rightarrow AH^+ \quad (1)$$




Changes in solvation free energies were calculated by subtracting the PBE0 free energy in vacuum from the PBE0 free energy calculated with the SMD solvent model. The latter was chosen because its documented good performance for solvation free energies, for instance, in a benchmark study on a set of 51 drug-like molecules (RMSD = 2.5 kcal/mol relative to experiment).[2] For the evaluation of the thermodynamic cycle, we used experimental values for the solvation free energy of hydronium ion, $H^+$, and water molecule,[3] and for the gas-phase free energy of $H^+$:[4] $\Delta G_{sol,1M}(H_2O)$ = -6.32 kcal/mol, $\Delta G_{sol,1M}(H_3O^+)$ = -110.3 kcal/mol, $\Delta G_{sol,1M}(H^+)$ = -265.9 kcal/mol, $\Delta G_{g,1atm}(H^+)$ = -6.28 kcal/mol. All energy values were converted to the standard state of 298 K and 1 M (1 mol/L). In the gas phase, equation (2), the change of 1 mole of ideal gas from 1 atm (24.46 L/mol) to 1 M gives rise to the following correction term:

$$\begin{aligned} \Delta G_{g,1M} &= \Delta G_{g,1atm} - T\Delta S \\ &= \Delta G_{g,1atm} + RT\ln\left(\frac{V_g}{V_{aq}}\right) \\ &= \Delta G_{g,1atm} + RT\ln(24.46) \\ &= \Delta G_{g,1atm} + 1.89 \text{ kcal/mol} \end{aligned} \quad (2)$$

Likewise, bringing water molecules from the concentration of 55.34 M in liquid water to 1M generates another correction term:

$$n \cdot \Delta G^*_{aq,1M}(H_2O) = -n \cdot RT\ln(55.34) = -2.38 \cdot n \text{ kcal/mol} \quad (3)$$

## Metal salt complexes in water

The complex formation of metal salts $MCl_x$ in water depends on many factors: the metal cation, temperature, the $pK_a$ of the complex, the pH of the solution, the available ligands (here: $H_2O$, $Cl^-$, $OH^-$, hydroxyl groups of glucose), and the ligand exchange rate. Under these diverse conditions, the investigated metal cations ($Al^{3+}$, $Mg^{2+}$, $Cr^{3+}$, $Fe^{3+}$, $Cu^{2+}$) can form different complexes in water, but they have in common that they can all form octahedral complexes with six water ligands (Figure 2).

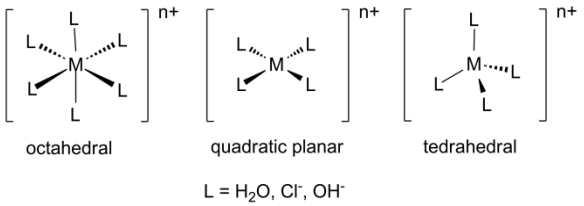



**Figure 2: Possible metal-ligand complexes of chloride salts in water.**

Which ligands are associated depends on the metal cation.[5] For $Cr^{3+}$ at high temperatures and for $Fe^{3+}$, it is common to exchange one to three water ligands for chloride ligands, whereas $Al^{3+}$ and $Mg^{2+}$ prefer water ligands. Copper(II) cations often have four ligands, favoring a tetrahedral (quadratic) arrangement for chloride (oxygen) ligands. The geometry of the actually formed copper(II) complexes depends on the concentration of salt in the solution, with tetrahedral $CuCl_4^{2-}$ complexes at high salt concentrations and $[Cu(H_2O)_2Cl_2]$ and $[Cu(H_2O)_6]^{2+}$ complexes at lower salt concentrations.

If a metal complex is acidic enough, the water ligands of the metal cation can act as proton donors, transforming a water ligand into a hydroxyl ion ligand (eq. 4).

$$[M(H_2O)_6]^{n+} + H_2O \rightarrow [M(H_2O)_5OH]^{m+} + H_3O^+ \quad (4)$$

Using a thermodynamic cycle the energy of a deprotonation reaction like equation (4) was calculated for metal cations $[M(H_2O)_6]^{n+}$ (Table 3). As expected, the computed energy ranges correlate qualitatively with the $pK_a$ of the metal cations. The values for $Cu^{2+}$ and $Al^{3+}$/$Cr^{3+}$ cations do not match the $pK_a$ values perfectly, as the thermodynamic cycle is not accurate enough for quantitative results in this case.[6] Complexes with exothermic reaction energies ($Cr^{3+}$, $Al^{3+}$, $Fe^{3+}$) are more likely to be found deprotonated in water. For example, iron(III) hexaqua-complexes are only stable at pH values lower than zero, and at higher pH values one to three water ligands are deprotonated.[5a],[7] Analogous relations are found for hexaaqua-aluminum(III) and chromium(III) complexes. As the experiment takes place in water at pH 7, deprotonation reactions become likely for these three metal complexes.

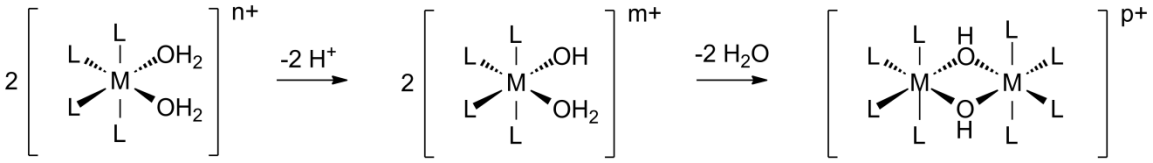
**Table 3: Free energies of deprotonation for $[M(H_2O)_6]^{n+}$ complexes in water calculated with a thermodynamic cycle (PBE0/6-31+G**).**

| Metal cation | $pK_a$ in water, 298 K | ΔG(deprot) / kcal $mol^{-1}$ |
|---|---|---|
| $Cu^{2+}$ | 8.0 | 26.3* |
| $H_2O$ | 15.7 | 23.5 |
| $Mg^{2+}$ | 11.4 | 20.3 |
| $Cr^{3+}$ | 4.1 | -0.5 |
| $Al^{3+}$ | 5.5 | -2.1 |
| $Fe^{3+}$ | 2.2 | -4.7 |

*calculated at the frozen geometry, since deprotonation leads to significant structural changes in $[Cu(H_2O)_6]^{2+}$

As can be seen in Table 3, the deprotonation reaction is endothermic for metal cation complexes that hardly catalyze the glucose to fructose isomerization ($Cu^{2+}$, $Mg^{2+}$, water), whereas for good catalysts ($Cr^{3+}$, $Al^{3+}$) and $Fe^{3+}$ the deprotonation reaction is exothermic. The influence of the Brønsted acidity of the different metal complexes will be discussed in the context of the mechanism in the Results section.

Depending on the pH of the solution binuclear complexes can also be formed (Scheme 1). Dimers can be found with single, double or triple chloride, hydroxo or oxo bridges, but most likely are doubly bridged hydroxo systems.[8] The higher the pH of the solution, the more probable is the formation of dimeric complexes, as dimers are predeceased by a deprotonation of water ligands. For example, the μ-hydroxyl bridged catalysts are found for chromium(III) and iron(III) complexes, and in low amounts also for aluminum(III) in aqueous systems.[5a],[7] Like the monomeric catalysts some dimers are able to bind to glucose: Extended x-ray absorption fine structure (EXAFS) spectroscopy found $Fe^{3+}$- dimers with the hydroxyl groups of glucose acting as ligands.[9] For the dimeric catalyst, only the rate determining steps were explored in the Results section.




**Scheme 1: Formation of a dimeric complexes with μ-water hydroxyl bridges.**

If sugar molecules are added to the metal complexes in water, they can act as bidentate ligands or can form hydrogen bonded complexes (Figure 3). The direct binding to glucose is entropically favored as two water ligands are detached (chelate effect). The position closest to the reaction centre for isomerization is the $O^1O^2$ position in glucose. For the $[M(H_2O)_4]^{n+}$ catalyst, the coordination sites $O^1O^2$, $O^2O^3$, $O^3O^4$, $O^3O^4$ and $O^4O^6$ were investigated, and their energies are displayed in Table 4. We did not perform such a study for $[M(H_2O)_6]^{n+}$, because a hydrogen bonded catalyst seems more unlikely in the high-pressure environment of the experimental setup since it has higher energies for the rate determining steps (see Results section). According to the literature, different percentages of complexed glucose are found for different metal cations in water: $Mg^{2+}$ 0%, $Fe^{3+}$ 8%, $Al^{3+}$ 9%, $Cr^{3+}$ 12% and $Cu^{2+}$ 14%.[10]

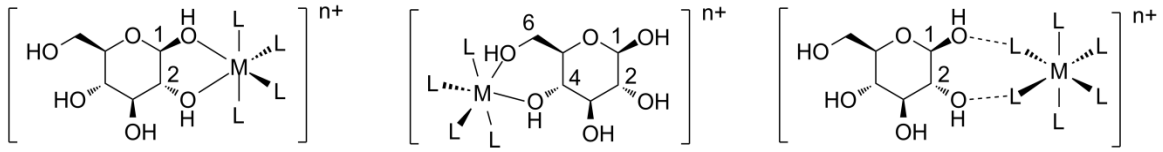



**Figure 3: Octahedral metal-ligand complexes with β-glucose as a bidentate ligand. $O^1O^2$ coordination (left), $O^4O^6$ coordination (middle) or attached to β-glucose via hydrogen bonds (right).**

**Table 4: Relative binding free energies between tetraaqua-metal complexes and α- and β-glucopyranose for different coordination sites (PBE0/6-31+G**, CPCM(water)).**

| Coordination | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
|---|---|---|---|---|---|
| α-glucose | $Al(H_2O)_4^{3+}$ | $Fe(H_2O)_4^{3+}$ | $Cr(H_2O)_4^{3+}$ | $Mg(H_2O)_4^{2+}$ | $Cu(H_2O)_4^{2+}$ |
| $O^1O^2$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $O^2O^3$ | -0.3 | -1.6 | -0.1 | -2.4 | -4.2 |
| $O^3O^4$ | 1.7 | -0.3 | -0.4 | -0.2 | -4.6 |
| $O^4O^6$ | -3.0 | -4.8 | -5.3 | -1.5 | -5.9 |
| $O^6O^5$ | 2.6 | -0.9 | -3.3 | 0.5 | -5.8 |
| β-glucose | $Al(H_2O)_4^{3+}$ | $Fe(H_2O)_4^{3+}$ | $Cr(H_2O)_4^{3+}$ | $Mg(H_2O)_4^{2+}$ | $Cu(H_2O)_4^{2+}$ |
| $O^1O^2$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| $O^2O^3$ | -3.0 | -3.9 | -4.3 | -0.9 | 0.4 |
| $O^3O^4$ | -0.4 | 0.3 | -1.3 | 0.7 | 0.3 |
| $O^4O^6$ | -5.3 | -5.5 | -6.1 | -0.7 | -1.1 |
| $O^6O^5$ | -5.8 | -5.2 | -5.1 | 0.9 | -1.0 |

According to Table 4, the $O^4O^6$ coordination is preferred in the majority of cases, as in this position a second six-membered ring can be formed between the metal complex and glucopyranose. The $O^1O^2$ and $O^3O^4$ coordination are least favorable for most metals. Nevertheless, the isomerization was investigated for $O^1O^2$ coordination of α-glucopyranose in this study. This coordination site is closest to the reactive centre of the glucose to fructose isomerization and should therefore help lower the barriers most efficiently. In addition, we note that the complexes with $O^1O^2$ coordination remain accessible because they are only 1-6 kcal/mol above the lowest-energy complex. In experiments with O1 methylated glucose, no isomerization was detected for $CrCl_2$ in ionic liquids.[11] This was taken as evidence that the isomerization can only be carried out if O1 is free for coordination, and hence only O1 coordination was regarded relevant in this study. The rate determining step (TS2) of theisomerization was investigated for the coordination site lowest in energy ($O^4O^6$), but no stable transition state was found.

In addition to the coordination site of glucose, the energy of the complex is also influenced by the ligand arrangement. Axial (ax1, ax2) and equatorial positions (eq1, eq2) were calculated for different numbers of chloride and hydroxyl ligands in the iron(III), chromium(III), and aluminum(III) complexes $[MO^1O^2(H_2O)_4]^{n+}$. For copper(II) the ligand positions in the complex $[CuO^1O^2(H_2O)Cl]^+$ were investigated. Since hydroxyl and chloride ligands are not likely for magnesium(II) complexes in water, no calculations were done with magnesium(II) and these ligands. Exemplary results are summarized in Table 5. For the subsequent mechanistic studies, we always chose the lowest-energy position. The energy of the rate determining steps was also spot-checked for different ligand positions, and the results (Table 7) agree mainly with the data in Table 5. In general the equatorial positions are lowest in energy, although the energy differences are only small for the different constitutions.

**Table 5: Relative free energies of α-glucose metal complexes with different chloride, hydroxide, and water ligands (PBE0/6-31+G**, CPCM(water)).**

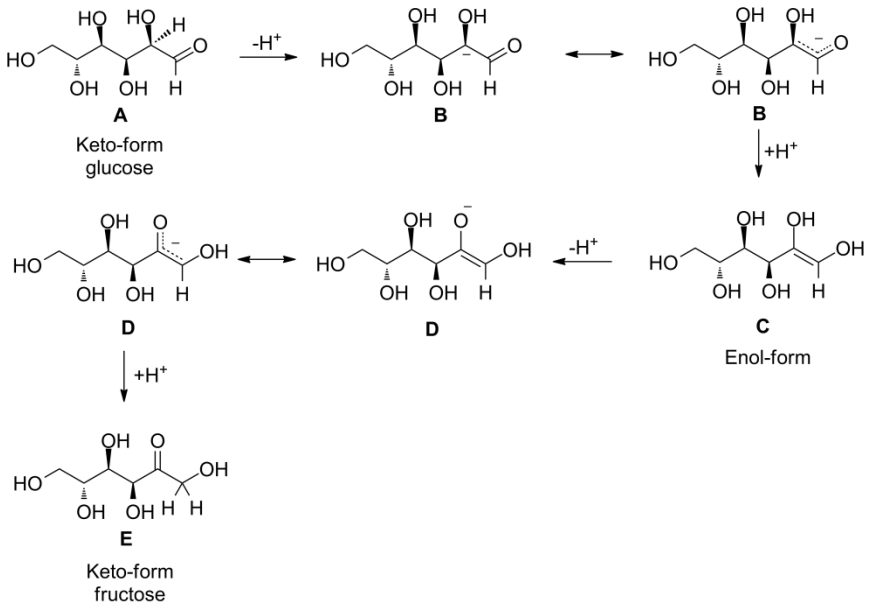
| complex | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
|---|---|---|---|
| catalyst → coordination ↓ | $Al(H_2O)_3Cl^{2+}$ | $Fe(H_2O)_3Cl^{2+}$ | $Cr(H_2O)_3Cl^{2+}$ |
| ax1 | 0.0 | 0.0 | 0.0 |
| ax2 | -1.0 | -0.5 | -0.1 |
| eq1 | -1.9 | -1.5 | -0.6 |
| eq2 | -1.6 | -2.6 | -2.0 |
| | $Al(H_2O)_2Cl_2^{+}$ | $Fe(H_2O)_2Cl_2^{+}$ | $Cr(H_2O)_2Cl_2^{+}$ |
| ax1-ax2 | -- | 0.0 | 0.0 |
| eq1-eq2 | -- | -3.1 | -1.6 |
| eq1-ax1 | -- | -0.8 | 0.8 |
| eq1-ax2 | -- | -1.9 | 1.2 |
| eq2-ax1 | -- | -1.5 | 1.2 |
| eq2-ax2 | -- | -1.1 | 0.1 |
| | $Al(H_2O)_3OH^{2+}$ | $Fe(H_2O)_3OH^{2+}$ | $Cr(H_2O)_3OH^{2+}$ |
| ax1 | 0.0 | 0.0 | 0.0 |
| ax2 | -2.1 | -0.9 | -1.0 |
| eq1 | -1.8 | -2.4 | -1.2 |
| eq2 | -3.3 | -3.2 | -2.8 |
| | | $Fe(H_2O)Cl_3$ | $Cr(H_2O)Cl_3$ |
| fac | -- | 0.0 | 0.0 |
| mer | -- | -2.2 | -1.4 |

Since it is hard to determine which of the complex configurations are most likely under the experimental conditions and how fast they change, the reaction mechanism was calculated for the most probable ligands for each metal cation.

In this study, all free energies refer to the sum of the free energies of $[M(H_2O)_6]^{n+}$ and α-glucopyranose. Free energies of reactants with chloride or hydroxyl ligands were adjusted to this reference by including the corresponding free energy of ligand exchange, as obtained from calculations at the same level of theory for water, hydronium, and chloride.

## Alternative pathway Keto-Enol-Tautomerization

An alternative to the hydrogen transfer TS2 is the keto-enol tautomerization. The tautomerization involves various de- and reprotonations via intermediates stabilized by charge delocalization in the keto- and enol-forms (Scheme 2). The relative reaction free energy for protonation and deprotonation reactions between the sugar molecule and the solvent were calculated with thermodynamic cycles (see above). This pathway was found to be higher in energy by 3 kcal/mol for the $[Al(H_2O)_4]^{3+}$ catalyzed pathway because of the higher energy for the proton addition from structure B to the enol-form C. Therefore this pathway was not further investigated. The H shift mechanism was also found to be preferred in enzymes according to the literature.[12]



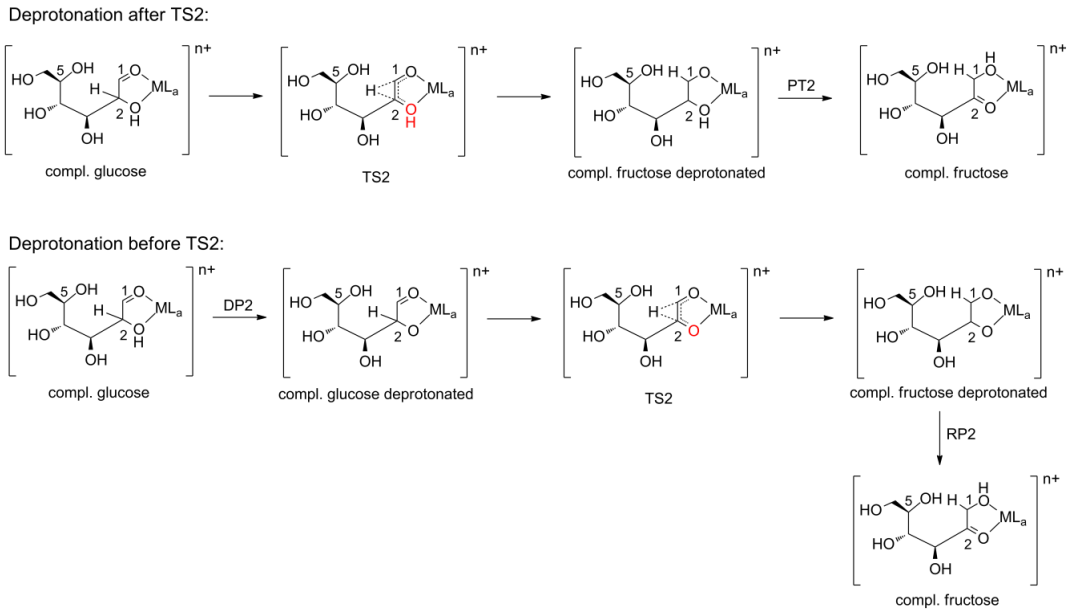

**Scheme 2: Keto-enol-Tautomerization as an alternative to the hydrogen shift TS2.**

**Table 6: Relative free Energies for the hydrogen transfer TS2 versus the Keto-Enol-Tautomerization. Energy references is glucosepyranose + $[Al(H_2O)_6]^{3+}$. Prot. barrier describes the energy needed for the protonation or deprotonation (PBE0/6-31+G**, CPCM(water)).**

| Hydrogen transfer | ΔG / kcal/mol | Keto-Enol-tautomerization | ΔG / kcal/mol |
|---|---|---|---|
| glucopyranose+$[Al(H_2O)_6]^{3+}$ | 0.0 | glucopyranose+$[Al(H_2O)_6]^{3+}$ | 0.0 |
| glucose-$[AlO^1O^2(H_2O)_4]^{3+}$ | 7.0 | glucose-$[AlO^1O^2(H_2O)_4]^{3+}$ = A | 7.0 |
| glucose deprot.-$[AlO^1O^2(H_2O)_4]^{3+}$ | 10.4 | B | 20.2 |
| | | prot. barrier | 25.9 |
| TS2 | 23.0 | C | 17.5 |
| fructose deprot.-$[AlO^1O^2(H_2O)_4]^{3+}$ | 6.4 | D | 17.8 |
| fructose-$[AlO^1O^2(H_2O)_4]^{3+}$ | -1.3 | E | -2.5 |

## Alternative pathway TS2-PT2 versus DP2-TS2-RP2:

One step of the glucose to fructose isomerization is a hydrogen shift (TS2), with a hydrogen atom being transferred from C2 to C1. The shift can be carried out with O2 being protonated or deprotonated (Scheme 3). Protonated and deprotonated forms of the transition states were calculated for examplary ligand constitutions and metals (Table 7). The lowest-energy form is always given in the Results section. If the transition state is protonated, the proton transfer from O2 to O1 occurs after the transition state (PT2). If the hydrogen transfer occurs in the deprotonated form, the O2 deprotonation (DP2) takes place before TS2 and the O1 protonation afterwards (RP2).




**Scheme 3: Possible intermediates before and after TS2, depending on the protonation state of O2 (marked in red) in the complexed glucose.**

**Table 7: Relative free energies for hydrogen transfer transition states with different ligand positions and protonation states (PBE0/6-31+G**, CPCM(water)).**

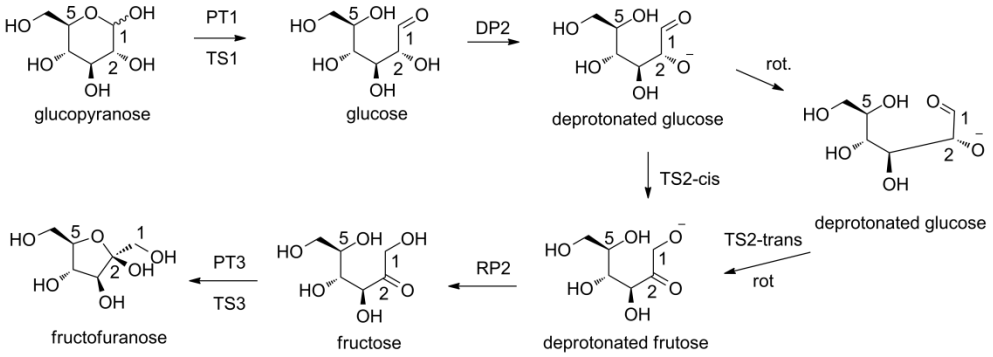
| TS2 | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
|---|---|---|---|
| catalyst → coordination ↓ | $Al(H_2O)_3Cl^{2+}$ | $Fe(H_2O)_3Cl^{2+}$ | $Cr(H_2O)_3Cl^{2+}$ |
| TS2 – ax1 | -- | -6.8 | -- |
| TS2 - ax1 - deprot | 10.4 | -1.3 | 1.2 |
| TS2 - ax2 | 13.3 | -8.0 | -- |
| TS2 – ax2 - deprot | -- | 3.4 | -- |
| TS2 - eq1 | 1.8 | -4.3 | -- |
| TS2 - eq1 - deprot | -- | -0.5 | -- |
| TS2 - eq2 | 10.7 | -5.4 | -4.0 |
| TS2 – eq2 - deprot | -- | -1.6 | 0.2 |
| | | $Fe(H_2O)Cl_3$ | |
| TS2 – eq1ax12 | -- | -42.2 | -- |
| TS2 – eq12ax2 | -- | -46.3 | -- |
| | $Al(H_2O)_3OH^{2+}$ | $Fe(H_2O)_3OH^{2+}$ | $Cr(H_2O)_3OH^{2+}$ |
| TS2 - ax1 - deprot | 55.8 | 44.9 | -- |
| TS2 - ax2 | 41.7 | -- | -- |
| TS2 – ax2 - deprot | -- | -- | 46.7 |
| TS2 - eq1 - deprot | 48.3 | -- | -- |
| TS2 - eq2 | 41.0 | 32.3 | 34.2 |
| TS2 – eq2 - deprot | 48.4 | 42.5 | 44.6 |
| | $Al(H_2O)_6^{3+}$ | | |
| TS2 | 24.4 | -- | -- |
| TS2 – deprot. | 40.6 | -- | -- |
| | $Al(H_2O)_4^{3+}$ | $Fe(H_2O)_4^{3+}$ | $Cr(H_2O)_4^{3+}$ |
| TS2 | 34.7 | 24.7 | 19.3 |
| TS2 – deprot. | 23.0 | 20.3 | 18.0 |
| | $Al_2(H_2O)_8(OH)_2^{4+}$ | | |
| TS2 | 57.8 | -- | -- |
| TS2 – deprot. | 40.1 | -- | -- |

# Detailed description of mechanisms

### Example 1: Glucopyranose to fructofuranose conversion mechanism without catalyst

To estimate the influence of the different metal catalysts, the uncatalyzed mechanism of the glucose to fructose conversion was calculated starting from α- and β-glucopyranose (Scheme 4, Figure 5, Table 8). Only the energies of PT1 and TS1 are different for the two anomeric forms of glucopyranose, as free rotation around the C1-C2 bond is assumed after ring opening.

All energies refer to α-glucopyranose.




**Scheme 4: Mechanism for the uncatalyzed pathway of glucose to fructose isomerization.**

The reaction starts with protonation of O5 and deprotonation of O1 (PT1) to facilitate the ring opening of the pyranose ring (Scheme 4, PT1). Overall, these de- and reprotonation reactions are endothermic by 38.1 kcal/mol for α-glucopyranose and by 33.7 kcal/mol for β-glucopyranose. After protonation of O5, a spontaneous ring opening by C1-O5 bond cleavage leads to glucose (TS1).

The next step is the deprotonation of O2 (DP2), which is necessary for the uncatalyzed mechanism as the negative charge on O2 eases the hydrogen transfer to C1 due to its positive inductive effect. The deprotonation energy was calculated to be 23.3 kcal/mol.

Thereafter, hydrogen transfer from C2 to C1 transforms the hydroxyl group at O2 into a keto group and O1 into a hydroxyl group (TS2, Figure 4). This reaction (Figure 4, TS2) can occur with the hydroxyl groups at the C1-C2 carbon bond in the *cis* (ΔG(TS2)=78.2 kcal/mol) or *trans* (ΔG(TS2)=88.9 kcal/mol) conformation. The *cis* transition state is lower in energy by ca. 10 kcal/mol, which might be due to the better charge delocalization in the more planar geometry of the *cis* structure (3° versus 17° in the O1-C1-C2-O2 dihedral angle). According to NBO analysis the electrons of the former C2-H bond are distributed between the $s_H$ orbital (0.799 e) of the transferred hydrogen atom and the two $\pi^*_{C1\text{-}O1}$ and $\pi^*_{C2\text{-}O2}$ orbitals (0.584 and 0.562 e). The hydrogen atom donates electron density into the $\pi^*_{C\text{-}O}$ orbitals. It carries a positive charge of 0.198 e.

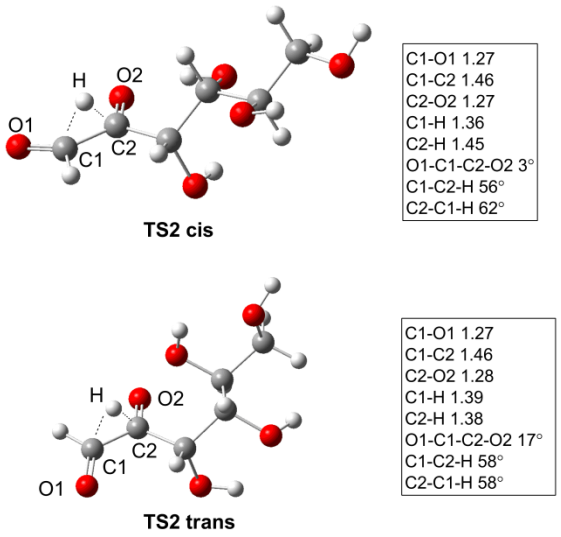



**Figure 4: Transition states for the uncatalyzed hydrogen atom transfer from C2 to C1 in the *cis* (top) and *trans* (bottom) conformation. Distances are given in Ångstrom (PBE0/6-31+G**, CPCM(water)).**

Beyond TS2, the O1 atom is protonated (RP2). Since the negative charge is mainly located at O1, this oxygen atom is a reasonable target for protonation, which is exothermic by -26.1 kcal/mol.

The last step involves ring closure (TS3) and proton transfer (PT3). The hydroxyl group at O5 attacks C2 and transfers the HO5 proton to O2, forming fructofuranose. The bond formation and the proton transfer occur in a concerted manner. After bond formation, 33.9 kcal/mol are needed for deprotonation of O5, and -41.5 kcal/mol are gained by protonation of O2.

The hydrogen atom transfer is the rate determining step, with an energy of 78.2 kcal/mol for TS2. It is clearly unfeasible even at 413 K. The overall reaction is endothermic by 1.5 kcal/mol. These findings are in agreement with experiments that show no conversion for the uncatalyzed reaction. A catalyst should lower the energies of PT1 and PT2 due to its Brønsted acidity as well as the transition state TS2 due to its Lewis acidity.

**Table 8: Relative free energies for the uncatalyzed reaction from glucopyranose to fructofuranose. The energy reference is α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
|---|---|---|
| structure | α-glucopyranose | β-glucopyranose |
| glucopyranose | 0.0 | -0.2 |
| PT1 – deprot. | 25.5 | 24.1 |
| PT1 – prot. | 38.1 | 33.4 |
| TS1 | | |
| glucose | 11.4 | 10.9 |
| DP2 | 34.2 | 34.8 |
| deprot. glucose | 72.5 | 77.8 |
| TS2 | 78.2 (cis) | 88.9 (trans) |
| deprot. fructose | 69.4 | 75.4 |
| RP2 | 43.3 | 49.3 |
| fructose | 7.2 | |
| TS3 | | |
| PT3 – deprot. | 41.1 | |
| PT3 – prot. | -0.3 | |
| fructofuranose | 1.5 | |

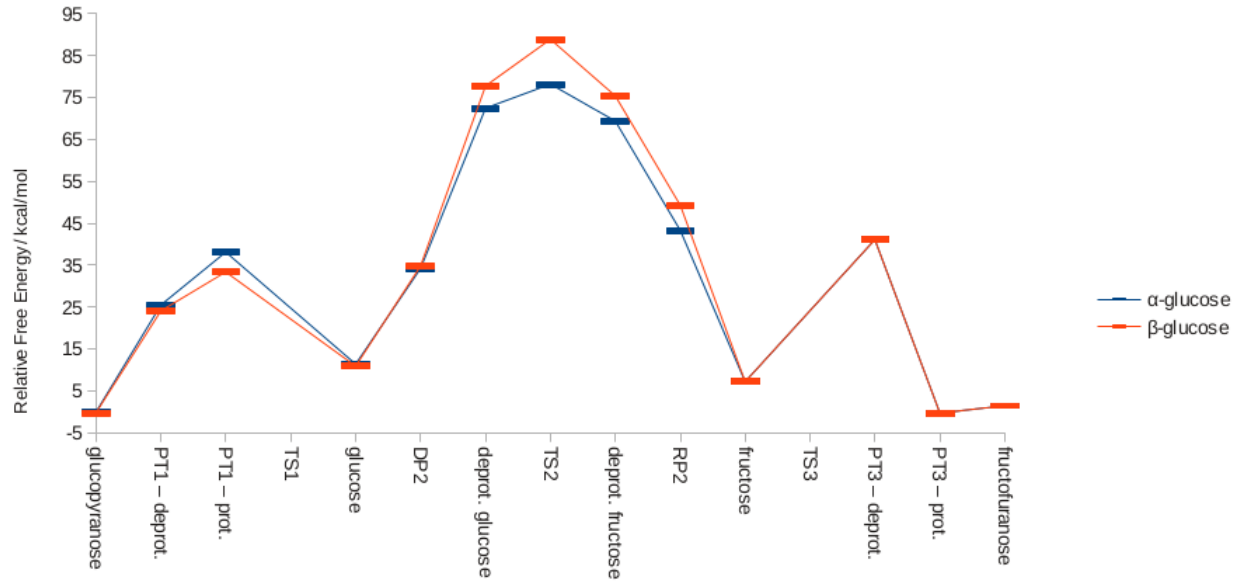



**Figure 5: Relative free energy profile in kcal mol$^{-1}$ for the uncatalyzed reaction pathway from glucopyranose to fructofuranose. Energy reference is α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

## Example 2: The $[Al(H_2O)_6]^{3+}$ catalyzed glucopyranose fructofuranose isomerization

One way to catalyze the isomerization is to attach the catalyst with hydrogen bonds to glucopyranose. As an example, we address $[Al(H_2O)_6]^{3+}$ as a catalyst (Table 9, Figure 10) pointing out similarities and differences with respect to the uncatalyzed reaction.

The first step is the formation of the weak $[Al(H_2O)_6]^{3+}$-α-glucopyranose complex, which stabilizes the system by -4.8 kcal/mol. In this complex, the aluminum(III) catalyst is coordinated via hydrogen bonds to the $O^1$ and $O^2$ hydroxyl groups of the glucopyranose molecule (Figure 6). Water ligands with hydrogen

bonds to glucopyranose [water(1) and water(2)] have somewhat shorter water-$Al^{3+}$ distances than the other water ligands without such hydrogen bonds. Compared to the uncatalyzed mechanism, the C1-O1 bond is elongated [Δd(C1-O1)=+0.02 Å], whereas the C1-O5 bond is shortened [Δd(C1-O5)=-0.02 Å].

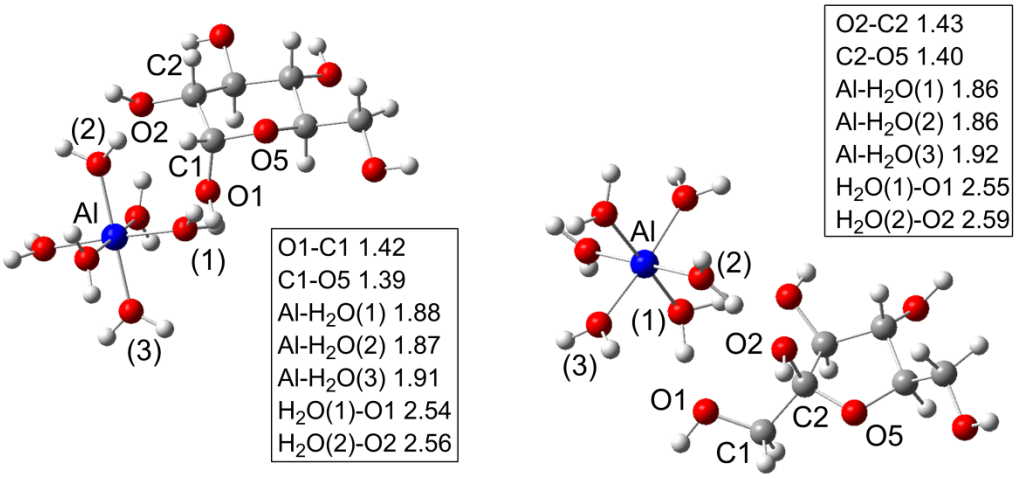



**Figure 6: Glucopyranose (left) and fructofuranose (right) form weak complexes with $[Al(H_2O)_6]^{3+}$. Distances are given in Ångstrom (PBE0/6-31+G**, CPCM(water)).**

In contrast to the uncatalyzed case, the initial deprotonation and reprotonation occur stepwise. The O1 deprotonation energy is -2.8 kcal/mol compared to 25.5 kcal/mol in the uncatalyzed mechanism, while the subsequent O5 protonation is endothermic by 19.8 kcal/mol (similar to the uncatalyzed case). The proton transfer (PT1) leads to a stable O5 protonated glucopyranose. The attached $Al^{3+}$-complex stabilizes the unprotonated hydroxyl group O1, and the C1-O5 bond is shorter than in the uncatalyzed case by 0.13 Å. After surmounting a small barrier of 8.3 kcal/mol, the ring is opened by C1-O5 cleavage (TS1) leading to glucose; TS1 is slightly lower than the energy of the previous minimum due to the inaccuracy of the thermal correction in combination with negative frequencies in Gaussian09.

The following step is the hydrogen atom transfer (TS2, Figure 7). With the $[Al(H_2O)_6]^{3+}$ catalyst, TS2 is 10 kcal/mol lower in energy when O2 is protonated rather than deprotonated. While the hydrogen atom is transferred from C2 to C1, O1 is protonated by one of the water ligands of the $Al^{3+}$ complex. Due to the complexation the C1-C2 bond is fixed in the *cis* position; this is advantageous considering that the *cis* transition state was already found to be lower in energy than its *trans* counterpart in the uncatalyzed mechanism (see above). NBO analysis shows that, unlike the uncatalyzed case, $s_H$ does not donate into the $\pi^*_{Cx\text{-}Oy}$ orbitals, but the $\pi^*_{Cx\text{-}Oy}$ orbitals donate into $s_H$ orbital, leading to an occupancy of 0.633e in $s_H$. The electronic population is 0.695e in the $\pi^*_{C1\text{-}O1}$ orbital and 0.611e in $\pi^*_{C2\text{-}O2}$. The positive charge on the hydrogen atom (0.365 e) is higher than in the uncatalyzed case. Electron density is also transferred into the $\sigma^*_{M\text{-}O}$ orbitals, which have an occupancy that is higher by 0.02 to 0.07e than in the unbound metal complex. The energy of TS2 is 24.4 kcal/mol.

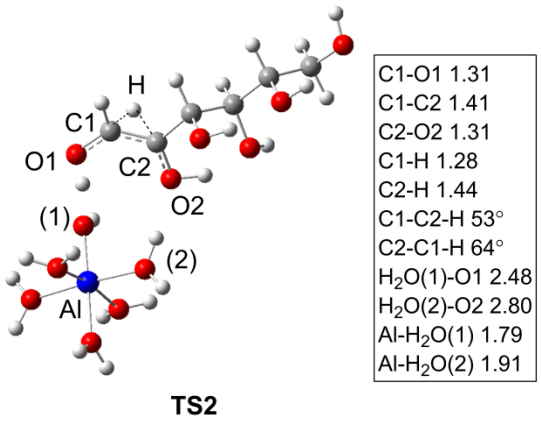



**Figure 7: Hydrogen atom transfer (TS2) with attached $[Al(H_2O)_6]^{3+}$ complex. Distances are given in Ångstrom (PBE0/6-31+G**, CPCM(water)).**

To obtain the open-chain fructose structure, another protons transfer (PT2) is needed, transferring the proton on O2 to the hydroxyl ligand (1) of the aluminum(III) complex. The deprotonation of O2 gains 19.1 kcal/mol, whereas the protonation of the hydroxyl ligand needs 4.3 kcal/mol.

With a keto group at O2, the structure is now prepared for forming fructofuranose via TS3. Like PT1 and TS1, TS3 and PT3 are stepwise processes. The open chain has to coil up, bringing O5 close to C2 for bond formation. The barrier for C2-O5 bond formation is 8.7 kcal/mol. The O5 deprotonation energy is -19 kcal/mol, the protonation of O2 needs 0.3 kcal/mol.

In the presence of the hydrogen bonded catalyst, the overall reaction becomes exothermic by 3.1 kcal/mol for the glucopyranose to fructofuranose conversion, whereas the uncatalyzed reaction is endothermic. However, the separation of catalyst and fructofuranose needs another 9.4 kcal/mol.

The rate determining transition state of the $[Al(H_2O)_6]^{3+}$ catalyzed isomerization mechanism is the same as in the uncatalyzed reaction: TS2, the hydrogen atom transfer. With ΔΔG(TS2) = 29 kcal/mol this barrier is feasible under the reaction conditions.

### Example 3: The $[AlO^1O^2(H_2O)_4]^{3+}$ catalyzed glucopyranose fructofuranose isomerization

An alternative to $[Al(H_2O)_6]^{3+}$ is the directly bonded complex $[AlO^1O^2(H_2O)_4]^{3+}$, which includes the hydroxyl groups O1 and O2 as ligands (Figure 11, Table 9). The isomerization mechanism with this catalyst will be compared to the uncatalyzed and the $[Al(H_2O)_6]^{3+}$ catalyzed mechanism.

The first step is the formation of the $[AlO^1O^2(H_2O)_4]^{3+}$-α-glucopyranose complex, in which two of the formerly coordinating water ligands are exchanged for the two hydroxyl groups at $O^1$ and $O^2$ of α-glucopyranose (Figure 8). The replaced water molecules are not included in the calculation explicitly for simplicity. The complex formation leads to a rise in energy of 2.3 kcal/mol. Due to the association of glucopyranose to the metal center, the chair conformer is slightly distorted bringing $O^1$ in a more equatorial and $O^2$ in a more axial position than in the uncatalyzed case. Continuing the previously observed trend, the C1-O1 bond is elongated [Δd(C1-O1)=+0.07 Å] and the C1-O5 bond is shortened [Δd(C1-O5)=-0.04 Å] compared to the hydrogen bonded complex $[Al(H_2O)_6]^{3+}$.

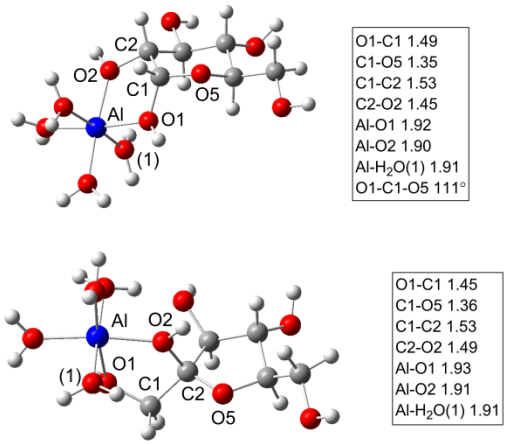



**Figure 8: Glucopyranose (top) and fructofuranose (bottom) form weak complexes with $[Al(H_2O)_4]^{3+}$. Distances are given in Ångstrom (PBE0/6-31+G**, CPCM(water)).**

Analogous to the $[Al(H_2O)_6]^{3+}$ mechanism, the initial deprotonation and reprotonation (TS1, PT1) occur stepwise. The deprotonation of O1 becomes even more exothermic with -8.1 kcal/mol, while the O5 protonation reaction energy is 19.1 kcal/mol and thus close to those obtained in examples 1 and 2. No transition state could be located for C1-O5 bond breaking, and scans show no barrier for this cleavage.

For the $[AlO^1O^2(H_2O)_4]^{3+}$ catalyzed isomerization, the sequence DP2, TS2, RP2 is lower in energy by 12 kcal/mol compared to the sequence TS2, PT2. The O2 deprotonation energy in DP2 is -8.8 kcal/mol. The structure of TS2 is different from the $[Al(H_2O)_6]^{3+}$ transition state (Figure 9). As O2 is deprotonated, there is no hydrogen bond between the hydroxyl group O3 and O2. Instead, the chain is bent so that water ligand (1) can form a hydrogen bond with O5. It was found that isomerizations with deprotonated O2 prefer ligand-O5 hydrogen bonds, whereas transition states with protonated O2 have O2-O3 hydrogen bonds. The NBO results for TS2 with the bonded catalyst are very similar to TS2 with the hydrogen bonded catalyst: Two electrons are delocalized between $\pi^*_{C1\text{-}O1}$ (0.640e), $\pi^*_{C2\text{-}O2}$ (0.714), and the s orbital of the hydrogen atom (0.650e). The charge on the hydrogen atom is 0.348e. As in the hydrogen bonded catalyst, electron density is pushed into the $\sigma^*_{M\text{-}O}$ orbitals. Their occupation is 0.02-0.03e higher compared to the $[Al(H_2O)_6]^{3+}$ catalyzed reaction path. The TS2 energy is only slightly lower than the one of $[Al(H_2O)_6]^{3+}$, with $\Delta G(TS2)$= 23.0 kcal/mol.

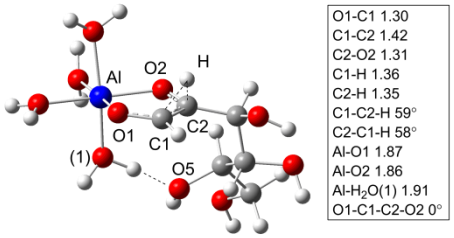



**Figure 9: Hydrogen atom transfer (TS2) with the $[Al(H_2O)_4]^{3+}$ complex. Distances are given in Ångstrom (PBE0/6-31+G**, CPCM(water)).**

After the H-shift O1 is protonated with an energy gain of -9.5 kcal/mol, leading to fructose.

In TS3 the O5-C2 bond is formed with a barrier of 7.0 kcal/mol. The following O5 deprotonation lowers the energy significantly by -18.2 kcal/mol, and the protonation of O2 raises the energy by 5.3 kcal/mol, leading to fructofuranose. The reaction from complexed glucopyranose to fructofuranose is exothermic by -16 kcal/mol. The fructofuranose catalyst separation needs 15 kcal/mol.

Like in examples 1 and 2, the hydrogen atom transfer (TS2) is the rate determining step. The energy for TS2 is lower than for the $[Al(H_2O)_6]^{3+}$ catalyzed reaction (23 vs. 29 kcal/mol). The fructofuranose-catalyst complex has an energy of -14 kcal/mol and is thus more stable than in the former examples.

The three examples show the following: The metal complex supports the proton transfers and the hydrogen atom shift, by accepting the electron density from deprotonated oxygen atoms and the broken C2-H bond. The deprotonation of O1 becomes more exothermic and the TS2 energy is lowered. The closer the metal cation to the C1-C2 bond, the better both are stabilized. How much this stabilization changes with different metal cations and ligands will now be investigated.

## Comparison with previous computational studies

Mu *et al.*[13] proposed a mechanism in ionic liquids that requires only direct proton transfers and keto-enol-tautomerization, similar to what we considered as an alternative mechanism (see Supporting Information). In our systems, such pathways were found to be higher in energy than our preferred pathway, and hence we did not investigate this alternative further.

The studies by van Santen[14] and Hensen[11, 15] in ionic liquids proposed a mechanism similar to ours. It differs only in that the proton transfers are not considered explicitly, with the focus being on the hydrogen shift (TS2). The authors found that O2 has to be deprotonated in TS2 (sequence DP2, TS2, RP2 in our study) and that the transition state barrier is lowered by using a dimeric complex. This is in contrast to our results in water: for some catalysts, the deprotonation before TS2 is unfavorable and a dimeric chromium(III) complex is higher in energy compared to the monomeric species. The differences might stem from the different stabilization of the stationary points by the solvent (ionic liquids vs. water).

Iron(II) and copper(II) catalysts yield a low conversion both in water and in ionic liquids. In the previous studies in ionic liquids, the inactivity of these metal cations was attributed to the inability of the $MCl_4^{2-}$ species to coordinate to the sugar, instead a nonselective deprotonation of glucose by the $Cl^-$ ligands was proposed. Again, there are differences to our results in water, where the formation of copper(II)- and iron(III)-glucose complexes is favorable (and only slightly unfavorable if hydroxyl ligands are attached).

These comparisons show that the solvent influences the reaction: While dimers and chloride ligands are helpful in the case of ionic liquids, they are obstructive in water. Despite these differences the rate determining step, a hydrogen shift, is the same in all studies.

## Overview over all mechanisms

In the preceding example section, two types of metal catalyzed reaction mechanisms were described. Metal catalysts that are bonded to glucose, catalyze the reaction in the same way as $[AlO^1O^2(H_2O)_4]^{3+}$, while hydrogen bonded catalysts take the same pathway as $[Al(H_2O)_6]^{3+}$. The sequence DP2, TS2, RP2 is found for the $[MO^1O^2(H_2O)_4]^{3+}$ and $M_2(H_2O)_8(OH)_2^{4+}$ catalysts, whereas the pathway TS2, PT2 applies for all other complexes and all magnesium(II) complexes. As an overview over the computational results, we present energy tables and energy diagrams of the lowest pathways for all metals with different ligand constitutions (Table 9 - Table 16, Figure 10 - Figure 18). Thereafter, the rate determining steps will be discussed in detail and compared for individual catalysts.

The complete mechanism was calculated for most of the complexes. In some cases, computations were performed only for the most important steps (TS2, PT1) and for the catalyst-glucopyranose and catalyst-fructofuranose complexes.

### Aluminum

**Table 9: Relative free energies for allisomerizations catalyzed by an aluminum(III) complex. Energy reference is the sum of the energies of the $[Al(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Al(H_2O)_6^{3+}$ | $Al(H_2O)_3OH^{2+}$ | $Al(H_2O)_3Cl^{2+}$ | | $Al(H_2O)_4^{3+}$ | $Al_2(H_2O)_8(OH)_2^{4+}$ |
|---|---|---|---|---|---|---|
| structure ↓ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | structure | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
| $Al(H_2O)_6^{3+}$ + glucop. | 0.0 | 0.0 | 0.0 | $Al(H_2O)_6^{3+}$ + glucop. | 0.0 | 0.0 |
| modified cat. ref. | | 15.7 | -21.3 | modified cat. ref. | | |
| compl. gluc. | -4.8 | 13.6 | -21.1 | compl. gluc. | 2.3 | |
| PT1 – deprot | -7.6 | 11.4 | -29.6 | PT1 – deprot | -5.8 | |
| PT1 – prot | 12.2 | 30.1 | -8.0 | PT1 – prot | 13.3 | |
| glucop. O5 prot. | 8.0 | 27.4 | -11.9 | glucopyranose O5 prot. | 11.0 | |
| TS1 | 8.3 | | | TS1 | | |
| glucose | -0.1 | 19.1 | -18.7 | glucose | 7.0 | |
| | | | | DP2 | -4.4 | |
| | | | | deprot. glucose | 10.4 | 36.0 |
| TS2 | 24.4 | 41.0 | 1.8 | TS2 | 23.0 | 40.1 |
| deprot. fructose | 13.8 | 28.9 | -12.6 | deprot. fructose | 6.4 | 10.0 |
| PT2 – deprot. | -5.3 | 11.9 | -28.5 | RP2 | 16.0 | |
| PT2 – prot. | -1.0 | 15.8 | -21.1 | | | |
| fructose | 2.5 | 9.7 | -20.4 | fructose | -1.3 | |
| TS3 | 8.7 | 17.5 | -13.8 | TS3 | 7.0 | |
| fructofuranose O5 prot. | 9.4 | 16.4 | -16.6 | fructofuranose O5 prot. | 0.7 | |
| PT 3 – deprot. | -9.5 | -1.5 | -35.3 | PT 3 – deprot. | -17.5 | |
| PT 3 – prot. | -9.8 | 0.5 | -26.3 | PT 3 – prot. | -12.2 | |
| fructofuranose | -7.9 | -0.5 | -32.8 | fructofuranose | -13.9 | |
| sep. compl. | | 17.2 | -19.8 | sep. compl. | | |
| $Al(H_2O)_6^{3+}$ + fructop. | 1.5 | 1.5 | 1.5 | $Al(H_2O)_6^{3+}$ + fructop. | 1.5 | 1.5 |

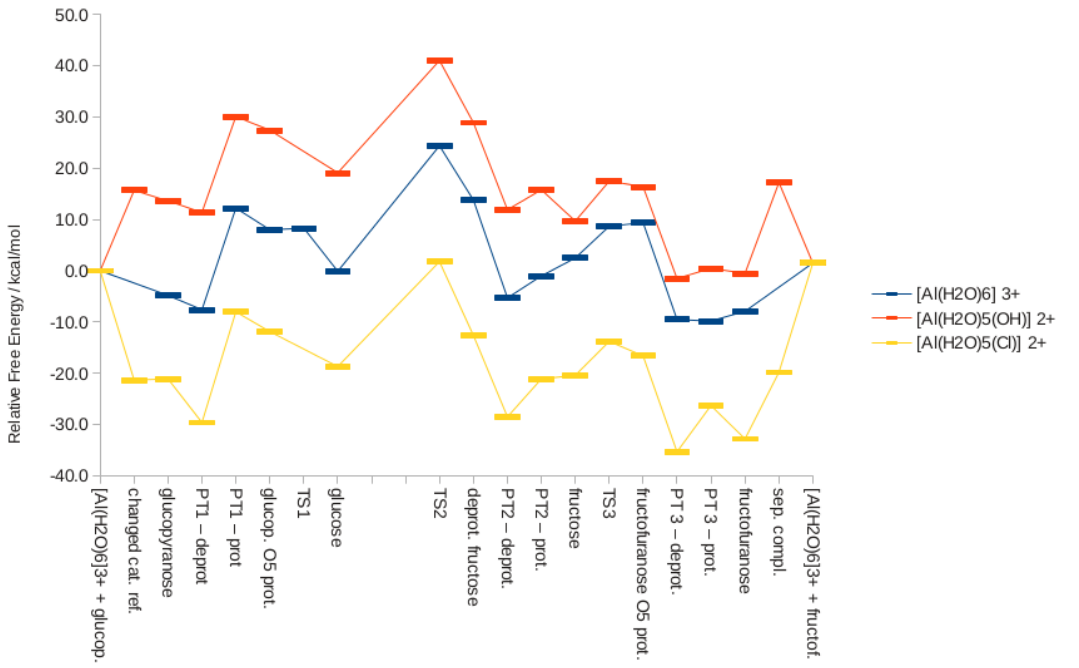



**Figure 10: Relative free energy profiles (kcal mol$^{-1}$) for isomerization catalyzed by an aluminum(III) complex, sequence TS2, PT2. Energy reference is the sum of the energies of the $[Al(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

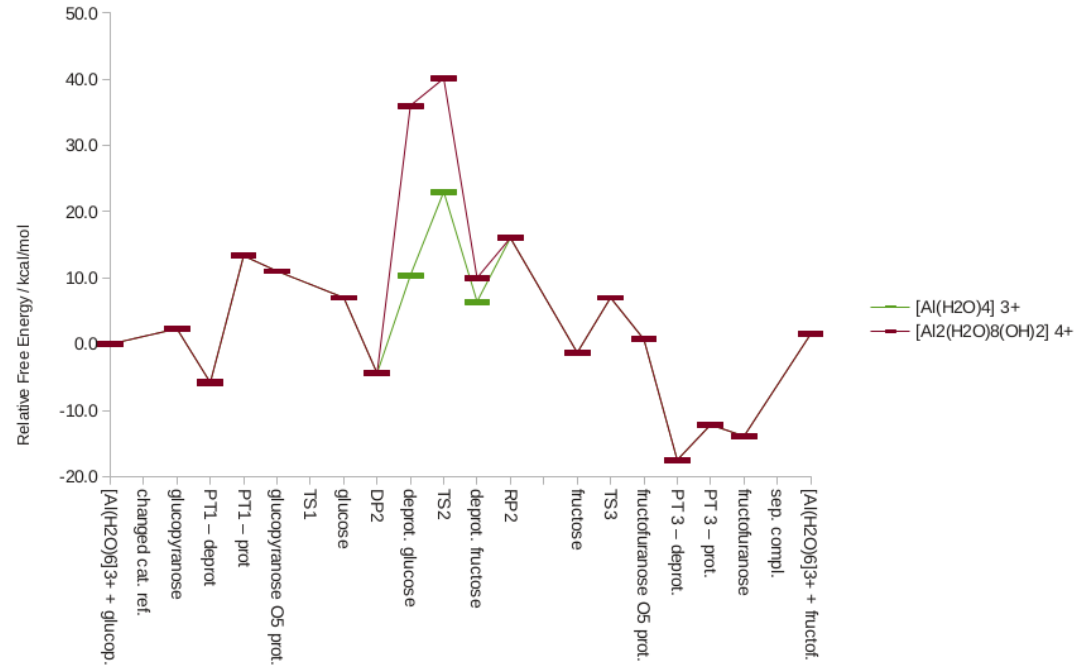



**Figure 11: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by an aluminum(III) complex, sequence DP2, TS2, RP2. Energy reference is the sum of the energies of the $[Al(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

## Chromium

**Table 10: Relative free energies for all isomerizations catalyzed by a chromium(III) complex, sequence: TS2, PT2. Energy reference is the sum of the energies of the $[Cr(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)_6^{3+}$ | $Cr(H_2O)_3OH^{2+}$ | $Cr(H_2O)_3Cl^{2+}$ | $Cr(H_2O)_2Cl_2^{+}$ | $Cr(H_2O)Cl_3$ |
|---|---|---|---|---|---|
| structure ↓ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ |
| $Cr(H_2O)_6^{3+}$ + glucop. | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| modified cat. ref. | | 8.5 | -27.8 | -50.2 | -64.4 |
| compl. gluc. | -4.4 | 6.4 | -29.9 | -53.5 | -65.4 |
| PT1 – deprot | -5.9 | 6.3 | -33.4 | -54.5 | -61.8 |
| PT1 – prot | 13.9 | 25.4 | -13.8 | -36.1 | -45.7 |
| glucop. O5 prot. | 5.5 | 20.5 | -17.3 | -37.1 | |
| TS1 | 7.2 | | | | |
| glucose | -2.6 | 7.0 | -24.9 | -46.2 | -61.7 |
| | | | | | |
| | | | | | |
| TS2 | 22.5 | 34.2 | -4.0 | -21.1 | -33.8 |
| deprot. fructose | 9.4 | 20.8 | -18.0 | -32.6 | -41.2 |
| PT2 – deprot. | -9.8 | 5.0 | -38.1 | -49.7 | |
| PT2 – prot. | -5.9 | 3.1 | -31.8 | -49.1 | |
| fructose | 2.4 | 8.3 | -32.6 | -50.1 | |
| TS3 | 6.8 | 16.1 | -22.7 | | |
| fructofuranose O5 prot. | 6.5 | 14.3 | -26.1 | -42.2 | |
| PT 3 – deprot. | -11.3 | 11.2 | -34.5 | -57.7 | |
| PT 3 – prot. | -10.7 | 9.6 | -30.7 | -59.0 | |
| fructofuranose | -11.6 | -4.5 | -43.4 | -61.5 | -69.8 |
| sep. compl. | | 9.9 | -26.4 | -48.7 | -63.0 |
| $Cr(H_2O)_6^{3+}$ + fructop. | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 |

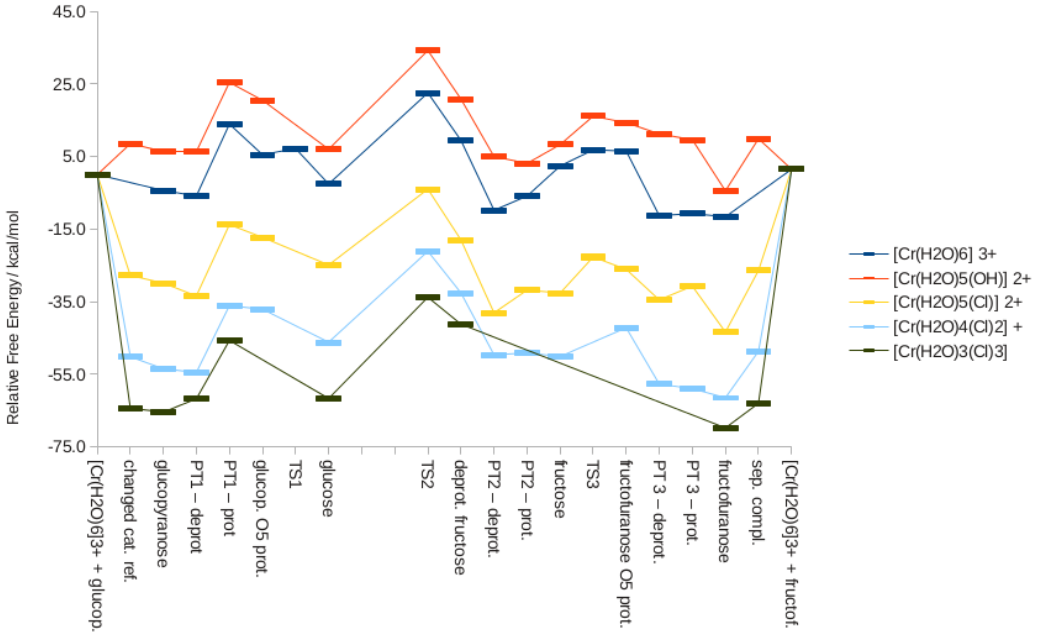



**Figure 12: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by a chromium(III) complex, sequence TS2, PT2. Energy reference is the sum of the energies of the $[Cr(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

**Table 11: Relative free energies for all isomerizations catalyzed by a chromium(III) complex, sequence: DP2,TS2, RP2. Energy reference is the sum of the energies of the $[Cr(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)_4^{3+}$ | $Cr_2(H_2O)_8(OH)_2^{4+}$ |
|---|---|---|
| structure ↓ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
| $Cr(H_2O)_6^{3+}$ + glucop. | 0.0 | 0.0 |
| modified cat. ref. | | |
| compl. gluc. | 0.7 | |
| PT1 – deprot | -4.1 | |
| PT1 – prot | 16.2 | |
| glucopyranose O5 prot. | 4.9 | |
| TS1 | | |
| glucose | 0.9 | |
| DP2 | -7.5 | |
| deprot. glucose | 4.4 | 32.3 |
| TS2 | 18.0 | 36.2 |
| deprot. fructose | 0.2 | 5.8 |
| RP2 | 9.3 | |
| fructose | -4.6 | |
| TS3 | 2.8 | |
| fructofuranose O5 prot. | -2.9 | |
| PT 3 – deprot. | -24.8 | |
| PT 3 – prot. | -18.6 | |
| fructofuranose | -16.8 | |
| sep. compl. | | |
| $Cr(H_2O)_6^{3+}$ + fructop. | 1.5 | 1.5 |

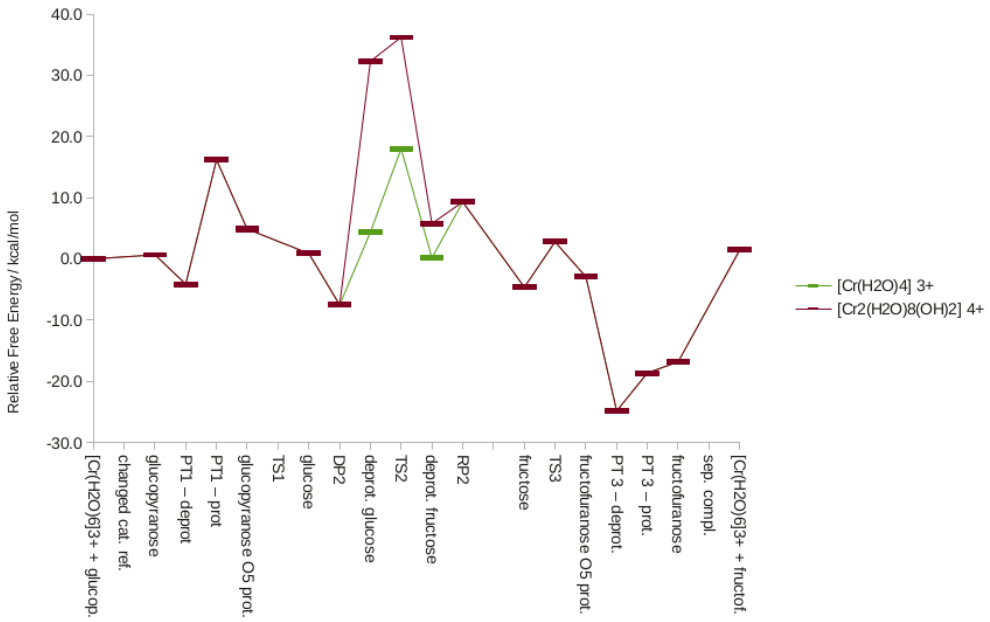



**Figure 13: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by a chromium(III) complex, sequence DP2, TS2, RP2. Energy reference is the sum of the energies of the $[Cr(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

## Iron

**Table 12: Relative free energies for all isomerizations catalyzed by an iron(III) complex, sequence: TS2, PT2. Energy reference is the sum of the energies of the $[Fe(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_3Cl^{2+}$ | $Fe(H_2O)_2(OH)Cl^{+}$ | $Fe(H_2O)_2Cl_2^{+}$ | $Fe(H_2O)(OH)Cl_2$ | $Fe(H_2O)Cl_3$ | $Fe(OH)Cl_3^{-}$ |
|---|---|---|---|---|---|---|
| structure ↓ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ |
| $Fe(H_2O)_6^{3+}$ + glucop. | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| modified cat. ref. | -31.8 | -31.8 | -55.2 | -55.2 | -72.3 | -70.1 |
| modified cat. ref. 2 | | -13.5 | | -28.4 | | |
| compl. gluc. | -35.6 | -21.0 | -60.4 | -35.1 | -73.9 | |
| PT1 – deprot | -40.0 | -18.4 | -61.8 | -30.7 | -70.2 | |
| PT1 – prot | -20.5 | -1.7 | -44.6 | -16.1 | -54.6 | |
| glucop. O5 prot. | -24.3 | | -44.3 | | | |
| TS1 | | | | | | |
| glucose | -27.8 | -12.9 | -51.7 | -27.3 | -68.1 | |
| | | | | | | |
| | | | | | | |
| TS2 | -5.4 | 10.2 | -25.0 | -3.6 | -42.2 | -9.6 |
| deprot. fructose | -13.8 | -3.6 | -49.0 | -15.9 | -58.8 | |
| PT2 – deprot. | -36.8 | | -59.7 | | | |
| PT2 – prot. | -29.8 | | -54.8 | | | |
| fructose | -37.2 | | -50.4 | | | |
| TS3 | | | | | | |
| fructofuranose O5 prot. | -29.3 | | -48.8 | | | |
| PT 3 – deprot. | -46.6 | | -59.1 | | | |
| PT 3 – prot. | -45.7 | | -58.1 | | | |
| fructofuranose | -46.4 | -25.9 | -65.3 | -36.5 | -73.9 | |
| sep. compl. | -30.3 | -12.0 | -53.7 | -27.0 | -70.9 | |
| $Fe(H_2O)_6^{3+}$ + fructop. | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | |

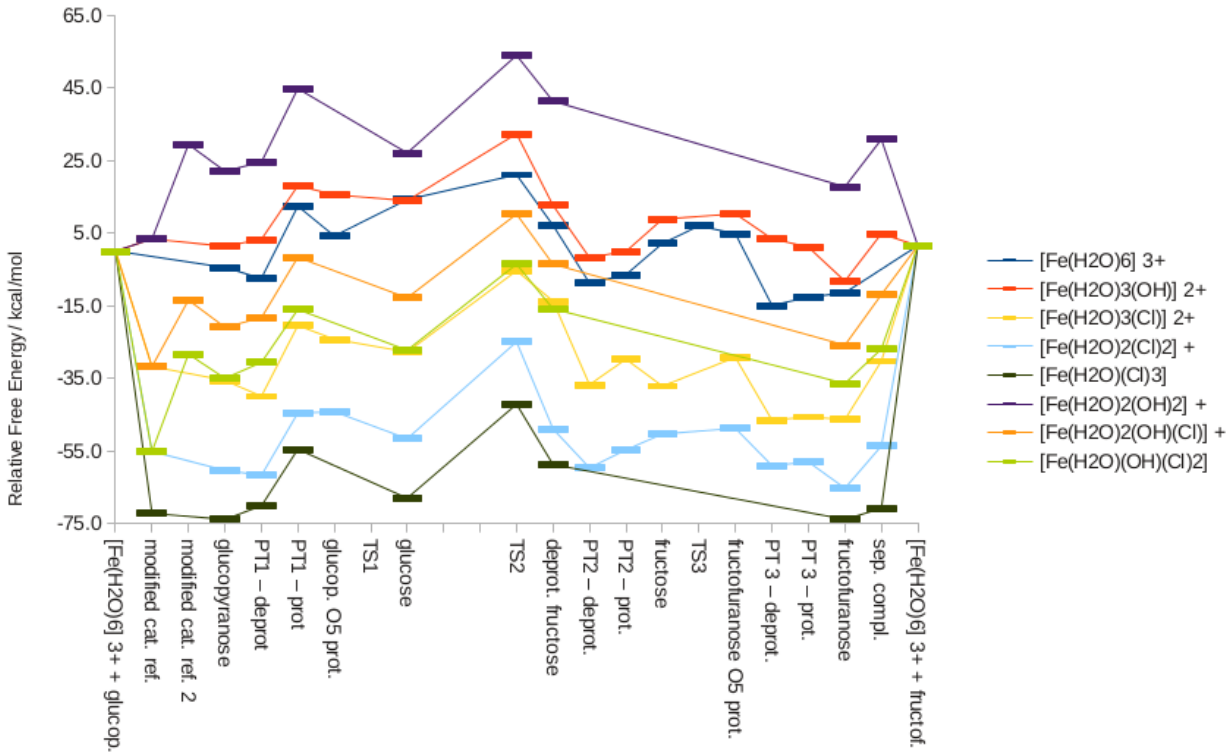



**Figure 14: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by an iron(III) complex, sequence TS2, PT2. Energy reference is the sum of the energies of the $[Fe(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

**Table 13: Relative free energies for all isomerizations catalyzed by an iron(III) complex, sequence: TS2, PT2 (left]; DP2, TS2, RP2 (right). Energy reference is the sum of the energies of the $[Fe(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_6^{3+}$ | $Fe(H_2O)_3OH^{2+}$ | $Fe(H_2O)_2(OH)_2^{+}$ | | $Fe(H_2O)_4^{3+}$ | $Fe_2(H_2O)_8(OH)_2^{4+}$ |
|---|---|---|---|---|---|---|
| structure ↓ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | structure | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ |
| $Fe(H_2O)_6^{3+}$ + glucop. | 0.0 | 0.0 | 0.0 | $Fe(H_2O)_6^{3+}$ + glucop. | 0.0 | 0.0 |
| modified cat. ref. | | 3.3 | 3.3 | modified cat. ref. | | |
| modified cat. ref. 2 | | | 29.4 | | | |
| compl. gluc. | -4.5 | 1.3 | 22.0 | compl. gluc. | 2.1 | |
| PT1 – deprot | -7.5 | 3.2 | 24.5 | PT1 – deprot | -6.9 | |
| PT1 – prot | 12.4 | 18.0 | 44.8 | PT1 – prot | 14.9 | |
| glucop. O5 prot. | 4.2 | 15.5 | | glucopyranose O5 prot. | 2.1 | |
| TS1 | | | | TS1 | 5.0 | |
| glucose | 14.2 | 13.9 | 27.0 | glucose | -5.1 | |
| | | | | DP2 | | |
| | | | | deprot. glucose | 1.6 | 23.5 |
| TS2 | 21.0 | 32.3 | 53.9 | TS2 | 20.3 | 31.1 |
| deprot. fructose | 7.1 | 12.6 | 41.3 | deprot. fructose | -2.8 | 3.1 |
| PT2 – deprot. | -8.8 | -1.8 | | RP2 | 7.8 | |
| PT2 – prot. | -6.5 | -0.1 | | | | |
| fructose | 2.1 | 8.8 | | fructose | -4.1 | |
| TS3 | 6.9 | | | TS3 | 3.8 | |
| fructofuranose O5 prot. | 4.8 | 10.3 | | fructofuranose O5 prot. | 1.6 | |
| PT 3 – deprot. | -15.0 | 3.4 | | PT 3 – deprot. | -21.1 | |
| PT 3 – prot. | -12.7 | 1.1 | | PT 3 – prot. | -15.4 | |
| fructofuranose | -11.5 | -8.3 | 17.7 | fructofuranose | -15.8 | |
| sep. compl. | | 4.8 | 30.8 | sep. compl. | | |
| $Fe(H_2O)_6^{3+}$ + fructop. | 1.5 | 1.5 | 1.5 | $Fe(H_2O)_6^{3+}$ + fructop. | 1.5 | 1.5 |

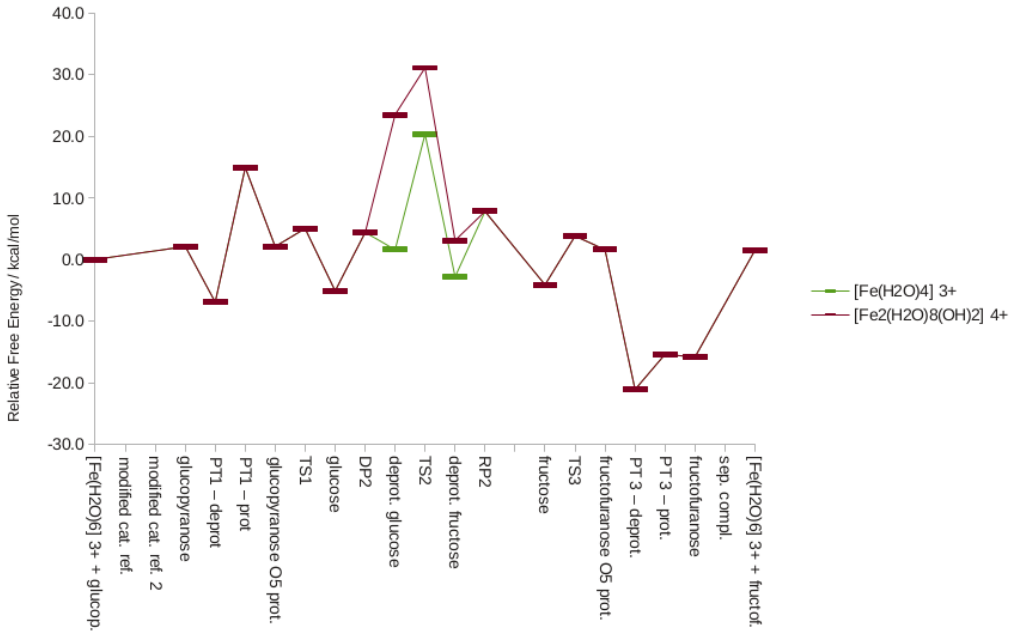



**Figure 15: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by an iron(III) complex, sequence DP2, TS2, RP2. Energy reference is the sum of the energies of the $[Fe(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

## Copper

**Table 14: Relative free energies for all isomerizations catalyzed by a copper(II) complex, sequence: TS2, PT2. Energy reference is the sum of the energies of the $[Cu(H_2O)_6]^{2+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cu(H_2O)_6^{2+}$ | $Cu(H_2O)Cl^{+}$ | $CuCl_2$ |
|---|---|---|---|
| structure ↓ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
| $Cu(H_2O)_6^{2+}$ + glucop. | 0.0 | 0.0 | 0.0 |
| modified cat. ref. | | -26.5 | -42.4 |
| compl. gluc. | -1.2 | -31.7 | -49.9 |
| PT1 – deprot | | -26.2 | -40.4 |
| PT1 – prot | | -11.6 | -21.3 |
| glucop. O5 prot. | | | |
| TS1 | | | |
| glucose | 4.9 | -20.1 | -37.8 |
| | | | |
| | | | |
| TS2 | 35.5 | 11.5 | -7.2 |
| deprot. fructose | 24.4 | 5.3 | -11.8 |
| PT2 – deprot. | | | |
| PT2 – prot. | | | |
| fructose | | | -45.9 |
| TS3 | | | |
| fructofuranose O5 prot. | | | |
| PT 3 – deprot. | | | |
| PT 3 – prot. | | | |
| fructofuranose | -3.5 | -31.6 | -49.2 |
| sep. compl. | | -25.1 | -40.9 |
| $Cu(H_2O)_6^{2+}$ + fructop. | 1.5 | 1.5 | 1.5 |

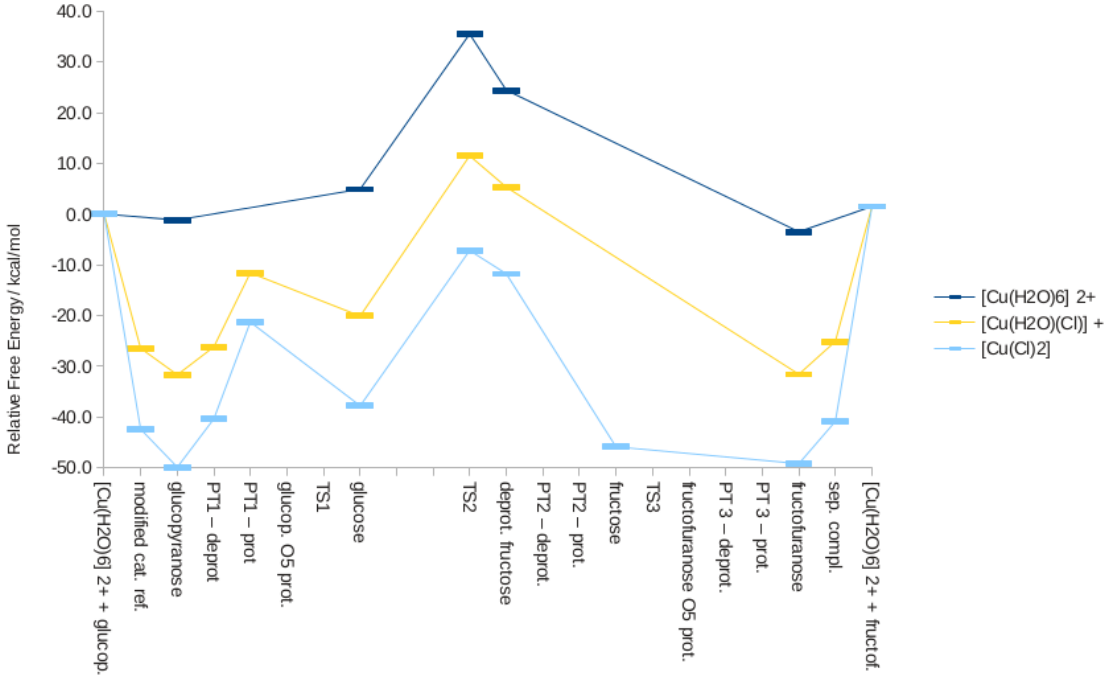



**Figure 16: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by a copper(II) complex, sequence TS2, PT2. Energy reference is the added energy of the $[Cu(H_2O)_6]^{3+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

**Table 15: Relative free energies for all isomerizations catalyzed by a copper(II) complex, sequence: DP2, TS2, RP2. Energy reference is the sum of the energies of the $[Cu(H_2O)_6]^{2+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cu(H_2O)_4^{2+}$ | $Cu(H_2O)_2^{2+}$ |
|---|---|---|
| structure ↓ | ΔG / kcal mol$^{-1}$ | ΔG / kcal mol$^{-1}$ |
| $Cu(H_2O)_6^{2+}$ + glucop. | 0.0 | 0.0 |
| modified cat. ref. | | |
| compl. gluc. | -0.4 | -7.4 |
| PT1 – deprot | -2.3 | -2.9 |
| PT1 – prot | | 12.7 |
| glucopyranose O5 prot. | | |
| TS1 | | |
| glucose | 2.5 | |
| DP2 | | |
| deprot. glucose | 23.0 | 18.6 |
| TS2 | 36.1 | 30.8 |
| deprot. fructose | 18.6 | 13.2 |
| RP2 | | |
| fructose | -4.6 | |
| TS3 | | |
| fructofuranose O5 prot. | | |
| PT 3 – deprot. | | |
| PT 3 – prot. | | |
| fructofuranose | -2.5 | -9.0 |
| sep. compl. | | |
| $Cu(H_2O)_6^{2+}$ + fructop. | 1.5 | 1.5 |

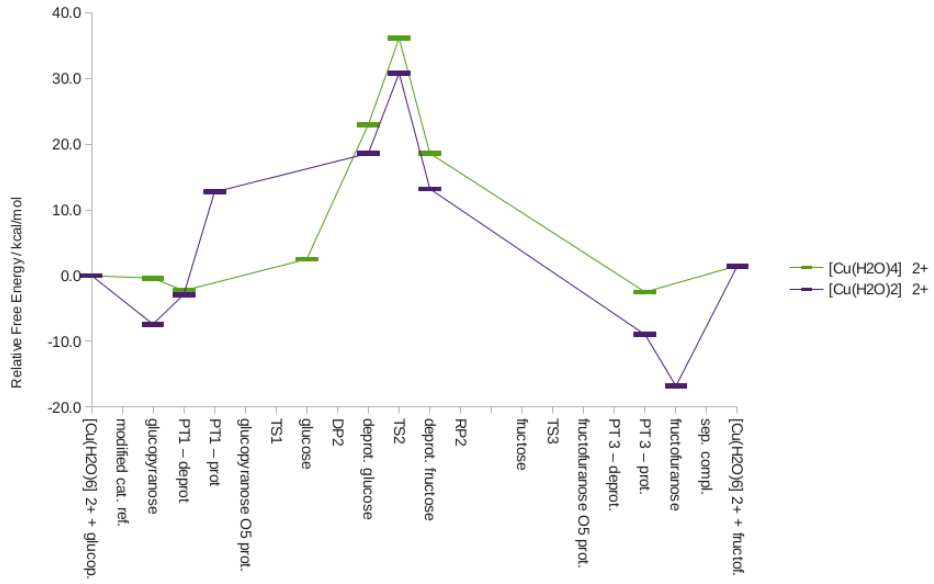



**Figure 17: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by a copper(II) complex, sequence DP2, TS2, RP2. Energy reference is the sum of the energies of the $[Cu(H_2O)_6]^{2+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

## Magnesium

**Table 16: Relative free energies for all isomerizations catalyzed by a magnesium(II) complex, sequence: TS2, PT2. Energy reference is the sum of the energies of the $[Mg(H_2O)_6]^{2+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $[Mg(H_2O)_6]^{2+}$ | $[Mg(H_2O)_4]^{2+}$ | | |
|---|---|---|---|---|
| structure ↓ | ΔG / kcal $mol^{-1}$ | ΔG / kcal $mol^{-1}$ | | |
| $Mg(H_2O)_6^{2+}$ + glucop. | 0.0 | 0.0 | | |
| modified cat. ref. | | | | |
| compl. gluc. | 2.1 | -0.7 | | |
| PT1 – deprot | 13.3 | 12.3 | | |
| PT1 – prot | 33.7 | 25.5 | | |
| glucop. O5 prot. | | | | |
| TS1 | | | | |
| glucose | 9.1 | 4.7 | | |
| | | | | |
| | | | | |
| TS2 | 40.1 | 34.4 | | |
| deprot. fructose | 34.0 | 27.5 | | |
| PT2 – deprot. | 19.4 | 31.3 | | |
| PT2 – prot. | 6.3 | 26.4 | | |
| fructose | 8.1 | 0.2 | | |
| TS3 | | | | |
| fructofuranose O5 prot. | 38.6 | 42.6 | | |
| PT 3 – deprot. | 24.7 | -2.8 | | |
| PT 3 – prot. | 11.9 | -14.9 | | |
| fructofuranose | 1.9 | -5.9 | | |
| sep. compl. | | | | |
| $Mg(H_2O)_6^{2+}$ + fructop. | 1.5 | 1.5 | | |

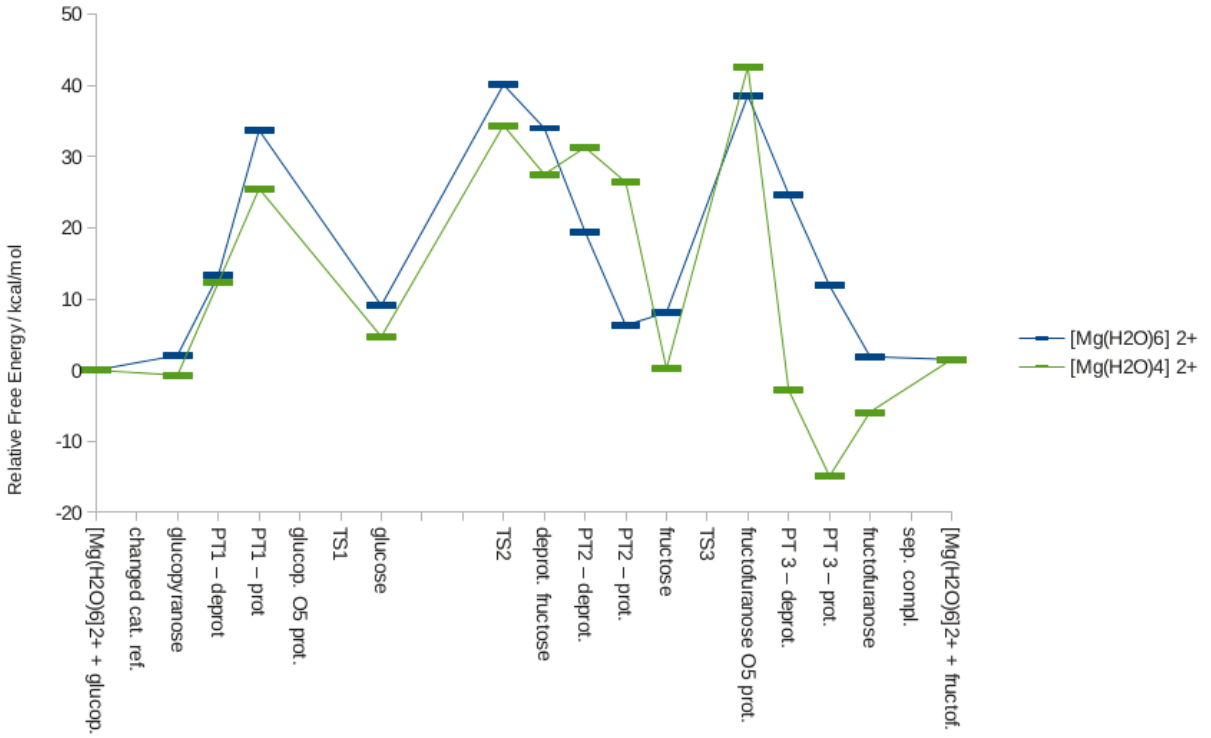



**Figure 18: Relative free energy profiles (kcal mol$^{-1}$) for isomerizations catalyzed by a magnesium(II) complex, sequence TS2, PT2. Energy reference is the sum of the energies of the $[Mg(H_2O)_6]^{2+}$ complex and α-glucopyranose (PBE0/6-31+G**, CPCM(water)).**

# Absolute energies of important structures

**Table 17: Absolute free energies, solvated and in vacuum, for the calculation of the deprotonation of $[M(H_2O)_6]^{n+}$ catalysts by a thermodynamic cycle.**

| | G_vacuum(PBE0/6-31+G**) / a.u. | G_solvated(PBE0/6-31+G**, SMD) / a.u. |
|---|---|---|
| $[Cu(H_2O)_6]^{2+}$ | -2097.559 | -2097.907 |
| $[Cu(H_2O)_5OH]^{+}$ | -2097.330 | -2097.435 |
| $H_3O^{+}$ | -76.610 | literature value (see above) |
| $H_2O$ | -76.346 | literature vale (see above) |
| $[Mg(H_2O)_6]^{2+}$ | -657.619 | -657.947 |
| $[Mg(H_2O)_5OH]^{+}$ | -657.362 | -657.484 |
| $[Cr(H_2O)_6]^{3+}$ | -1501.196 | -1501.947 |
| $[Cr(H_2O)_5OH]^{2+}$ | -1501.151 | -1501.517 |
| $[Al(H_2O)_6]^{3+}$ | -699.379 | -700.110 |
| $[Al(H_2O)_5OH]^{2+}$ | -699.327 | -699.682 |
| $[Fe(H_2O)_6]^{3+}$ | -1720.334 | -1721.093 |
| $[Fe\ (H_2O)_5OH]^{2+}$ | -1720.302 | -1720.670 |

**Table 18: Absolute free energies of different functionals for the isomerization with $[AlO^1O^2(H_2O)_4]^{3+}$ catalyst comparison with used method.**

| | G(B3LYP/6-31+G**) / a.u. | G(M06/6-31+G**) / a.u. | G(PBE0/6-311+G**) / a.u. |
|---|---|---|---|
| glucopyranose | -687.087 | -686.729 | -686.551 |
| fructofuranose | -687.083 | -686.725 | -686.548 |
| $[Al(H_2O)_6]^{3+}$ | -700.656 | -700.432 | -700.217 |
| $H_2O$ | -76.439 | -76.403 | -76.382 |
| $H_3O^+$ | -76.816 | -76.779 | -76.761 |
| glucosepyranose + $[Al(H_2O)_6]^{3+}$ | -1387.743 | -1387.161 | -1386.767 |
| glucopyranose | -1234.854 | -1234.350 | -1234.002 |
| PT1 | | | |
| glucopyranose O5 prot. | -1234.847 | -1234.338 | -1233.992 |
| TS1 | | | |
| glucose | -1234.856 | -1234.342 | -1233.996 |
| DP2 | | | |
| deprot. glucose | -1234.469 | -1233.962 | -1233.610 |
| TS2 | -1234.445 | -1233.937 | -1233.591 |
| deprot. fructose | -1234.474 | -1233.965 | -1233.616 |
| RP2 | | | |
| fructose | -1234.867 | -1234.359 | -1234.008 |
| TS3 | -1234.855 | -1234.345 | -1233.996 |
| fructofuranose O5 prot. | -1234.855 | -1234.348 | -1234.004 |
| PT3 | | | |
| fructofuranose | -1234.864 | -1234.357 | -1234.012 |
| fructofuranose +$[Al(H_2O)_6]^{3+}$ | -1387.739 | -1387.157 | -1386.765 |

**Table 19: Absolut energies at 413 K and 80 bar for critical steps in the glucose-fructose isomerization with selected $Al^{3+}$ and $Fe^{3+}$ catalysts (PBE0/6-31+G**, CPCM(water)).**

| | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|
| glucose | -686.502 | -686.304 | -686.280 | -686.359 |
| fructose | -686.498 | -686.301 | -686.276 | -686.357 |
| $[Al(H_2O)_6]^{3+}$ | -700.153 | -699.996 | -1083.877 | -700.050 |
| $[Al(H_2O)_5Cl]^{2+}$ | -1084.034 | -1083.903 | -1083.877 | -1083.958 |
| $[Fe(H_2O)_6]^{3+}$ | -1721.088 | -1720.937 | -1720.907 | -1720.999 |
| $[Fe(H_2O)_5Cl]^{2+}$ | -2104.989 | -2104.861 | -2104.833 | -2104.924 |
| $H_2O$ | -76.357 | -76.336 | -76.331 | -76.357 |
| $H_3O^+$ | -76.750 | -76.714 | -76.709 | -76.737 |
| $Cl^-$ | -460.213 | -460.213 | -460.210 | -460.230 |
| glucopyranose-$[Al(H_2O)_6]^{3+}$ | -1386.685 | -1386.327 | -1386.276 | -1386.415 |
| glucopyranose-$[AlO^1O^2(H_2O)_4]^{3+}$ | -1233.920 | -1233.614 | -1233.571 | -1233.691 |
| glucopyranose-$[AlO^1O^2(H_2O)_3Cl]^{2+}$ | -1617.809 | -1617.526 | -1617.485 | -1617.600 |
| TS2-$[Al(H_2O)_6]^{3+}$ | -1386.630 | -1386.279 | -1386.228 | -1386.369 |
| TS2-$[AlO^1O^2(H_2O)_4]^{3+}$ | -1233.490 | -1233.202 | -1233.161 | -1233.277 |
| TS2-$[AlO^1O^2(H_2O)_3Cl]^{2+}$ | -1617.761 | -1617.488 | -1617.446 | -1617.565 |
| fructofuranose-$[AlO^1O^2(H_2O)_3Cl]^{2+}$ | -1617.83 | -1617.55 | -1617.51 | -1617.62 |
| glucopyranose-$[Fe(H_2O)_6]^{3+}$ | -2407.620 | -2407.268 | -2407.215 | -2407.363 |
| glucopyranose-$[FeO^1O^2(H_2O)_4]^{3+}$ | -2254.861 | -2254.558 | -2254.513 | -2254.638 |
| glucopyranose-$[FeO^1O^2(H_2O)_3Cl]^{2+}$ | -2638.77 | -2638.49 | -2638.45 | -2638.57 |
| TS2-$[Fe(H_2O)_6]^{3+}$ | -2407.564 | -2407.216 | -2407.162 | -2407.314 |
| TS2-$[FeO^1O^2(H_2O)_4]^{3+}$ | -2254.434 | -2254.149 | -2254.106 | -2254.229 |
| TS2-$[FeO^1O^2(H_2O)_3Cl]^{2+}$ | -2638.713 | -2638.441 | -2638.398 | -2638.525 |
| fructofuranose-$[FeO^1O^2(H_2O)_3Cl]^{2+}$ | -2638.79 | -2638.51 | -2638.47 | -2638.59 |

**Table 20: Absolute binding energies between tetraaqua-metal complexes and α-glucopyranose for different coordination sites (PBE0/6-31+G**, CPCM(water)).**

| α-glucopyranose | coordination site | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $[Al(H_2O)_4]^{3+}$ | $O^1O^2$ | -1233.920 | -1233.614 | -1233.589 | -1233.664 |
| | $O^2O^3$ | -1233.92486628 | -1233.616911 | -1233.593087 | -1233.665215 |
| | $O^3O^4$ | -1233.92083493 | -1233.613066 | -1233.588966 | -1233.661981 |
| | $O^4O^6$ | -1233.93052670 | -1233.621721 | -1233.598082 | -1233.669538 |
| | $O^5O^6$ | -1233.92309188 | -1233.613300 | -1233.589979 | -1233.660552 |
| $[Fe(H_2O)_4]^{3+}$ | $O^1O^2$ | -2254.861 | -2254.558 | -2254.532 | -2254.610 |
| | $O^2O^3$ | -2254.86637811 | -2254.561403 | -2254.536585 | -2254.612737 |
| | $O^3O^4$ | -2254.86218636 | -2254.557711 | -2254.532388 | -2254.610769 |
| | $O^4O^6$ | -2254.87124223 | -2254.566390 | -2254.541386 | -2254.617832 |
| | $O^5O^6$ | -2254.86336128 | -2254.559149 | -2254.533768 | -2254.611663 |
| $[Cr(H_2O)_4]^{3+}$ | $O^1O^2$ | -2035.731 | -2035.424 | -2035.400 | -2035.475 |
| | $O^2O^3$ | -2035.73204409 | -2035.424454 | -2035.400401 | -2035.475435 |
| | $O^3O^4$ | -2035.73253568 | -2035.425346 | -2035.401188 | -2035.475878 |
| | $O^4O^6$ | -2035.74127933 | -2035.433248 | -2035.409439 | -2035.483615 |
| | $O^5O^6$ | -2035.73591048 | -2035.429116 | -2035.404703 | -2035.480479 |
| $[Mg(H_2O)_4]^{2+}$ | $O^1O^2$ | -1191.786 | -1191.485 | -1191.457 | -1191.539 |
| | $O^2O^3$ | -1191.78893433 | -1191.488128 | -1191.460445 | -1191.543260 |
| | $O^3O^4$ | -1191.78670280 | -1191.485220 | -1191.457760 | -1191.539773 |
| | $O^4O^6$ | -1191.79185344 | -1191.489092 | -1191.462424 | -1191.541804 |
| | $O^5O^6$ | -1191.78989099 | -1191.486784 | -1191.460319 | -1191.538677 |
| $[Cu(H_2O)_4]^{2+}$ | $O^1O^2$ | -2631.720 | -2631.418 | -2631.391 | -2631.474 |
| | $O^2O^3$ | -2631.72930934 | -2631.426090 | -2631.399568 | -2631.480749 |
| | $O^3O^4$ | -2631.73159889 | -2631.427519 | -2631.401589 | -2631.481358 |
| | $O^4O^6$ | -2631.73314918 | -2631.429816 | -2631.403482 | -2631.483439 |
| | $O^5O^6$ | -2631.73461720 | -2631.430462 | -2631.404651 | -2631.483338 |

**Table 21: Absolute binding energies between tetraaqua-metal complexes and β-glucopyranose for different coordination sites (PBE0/6-31+G**, CPCM(water)).**

| β-glucopyranose | coordination site | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $[Al(H_2O)_4]^{3+}$ | $O^1O^2$ | -1233.91368131 | -1233.606777 | -1233.582327 | -1233.656375 |
| | $O^2O^3$ | -1233.91946074 | -1233.612345 | -1233.588232 | -1233.661150 |
| | $O^3O^4$ | -1233.91533046 | -1233.608083 | -1233.583858 | -1233.657009 |
| | $O^4O^6$ | -1233.92552784 | -1233.616963 | -1233.593231 | -1233.664770 |
| | $O^5O^6$ | -1233.92517332 | -1233.617390 | -1233.593613 | -1233.665597 |
| $[Fe(H_2O)_4]^{3+}$ | $O^1O^2$ | -2254.85458427 | -2254.552417 | -2254.526186 | -2254.606767 |
| | $O^2O^3$ | -2254.86044820 | -2254.558122 | -2254.531884 | -2254.612967 |
| | $O^3O^4$ | -2254.85674033 | -2254.553290 | -2254.527642 | -2254.606270 |
| | $O^4O^6$ | -2254.86613380 | -2254.562551 | -2254.536994 | -2254.615453 |
| | $O^5O^6$ | -2254.86586756 | -2254.562240 | -2254.536706 | -2254.615038 |
| $[Cr(H_2O)_4]^{3+}$ | $O^1O^2$ | -2035.72467301 | -2035.418785 | -2035.394220 | -2035.469488 |
| | $O^2O^3$ | -2035.73007941 | -2035.424270 | -2035.399713 | -2035.476340 |
| | $O^3O^4$ | -2035.72690707 | -2035.420767 | -2035.396270 | -2035.471526 |
| | $O^4O^6$ | -2035.73631767 | -2035.428981 | -2035.404939 | -2035.479179 |
| | $O^5O^6$ | -2035.73584391 | -2035.428428 | -2035.404750 | -2035.477675 |
| $[Mg(H_2O)_4]^{2+}$ | $O^1O^2$ | -1191.78266651 | -1191.482118 | -1191.454361 | -1191.536936 |
| | $O^2O^3$ | -1191.78429280 | -1191.483647 | -1191.455986 | -1191.538309 |
| | $O^3O^4$ | -1191.78213422 | -1191.481349 | -1191.453683 | -1191.535888 |
| | $O^4O^6$ | -1191.78743220 | -1191.485205 | -1191.458389 | -1191.538056 |
| | $O^5O^6$ | -1191.78349407 | -1191.481720 | -1191.454557 | -1191.535573 |
| $[Cu(H_2O)_4]^{2+}$ | $O^1O^2$ | -2631.72679291 | -2631.423496 | -2631.397163 | -2631.477429 |
| | $O^2O^3$ | -2631.72634434 | -2631.423126 | -2631.396854 | -2631.476765 |
| | $O^3O^4$ | -2631.72620035 | -2631.422689 | -2631.396511 | -2631.476926 |
| | $O^4O^6$ | -2631.72863324 | -2631.425563 | -2631.399133 | -2631.479196 |
| | $O^5O^6$ | -2631.73035257 | -2631.426007 | -2631.400292 | -2631.479010 |

**Table 22: Absolute energies of different aluminum(III)-complexes (PBE0/6-31+G**, CPCM(water)).**

| | non-water ligand position | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $[Al(H_2O)_4]^{3+}$ | | -547.322 | -547.217 | -547.206 | -547.250 |
| $[Al(H_2O)_6]^{3+}$ | | -700.153 | -699.996 | -699.980 | -700.033 |
| $[Al(H_2O)_5Cl]^{2+}$ | | -1084.03 | -1083.903 | -1083.887 | -1083.941 |
| $[Al(H_2O)_5OH]^{2+}$ | | -699.737 | -699.592 | -699.577 | -699.629 |
| α-glucopyranose-$[Al(H_2O)_6]^{3+}$ | | -1386.685 | -1386.327 | -1386.298 | -1386.384 |
| α-glucopyranose-$[Al(H_2O)_4]^{3+}$ | | -1233.920 | -1233.614 | -1233.589 | -1233.664 |
| α-glucopyranose-$[Al(H_2O)_5Cl]^{2+}$ | ax1 | -1617.805 | -1617.523 | -1617.499 | -1617.572 |
| | ax2 | -1617.806 | -1617.525 | -1617.501 | -1617.574 |
| | eq1 | -2419.627 | -2419.345 | -2419.322 | -1617.575 |
| | eq2 | -1617.809 | -1617.526 | -1617.503 | -1617.575 |
| α-glucopyranose-$[Al(H_2O)_5OH]^{2+}$ | ax1 | -1233.507 | -1233.213 | -1233.189 | -1233.262 |
| | ax2 | -1233.511 | -1233.216 | -1233.193 | -1233.266 |
| | eq1 | -1233.511 | -1233.217 | -1233.193 | -1233.265 |
| | eq2 | -1233.513 | -1233.219 | -1233.195 | -1233.268 |

**Table 23: Absolute energies of different chromium(III)-complexes (PBE0/6-31+G**, CPCM(water)).**

| | non-water ligand position | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $[Cr(H_2O)_6]^{3+}$ | dublett | -1501.917 | -1501.762 | -1501.746 | -1501.801 |
| $[Cr(H_2O)_6]^{3+}$ | quartett | -1501.959 | -1501.803 | -1501.787 | -1501.842 |
| $[Cr(H_2O)_5Cl]^{2+}$ | | -1885.852 | -1885.721 | -1885.705 | -1885.761 |
| $[Cr(H_2O)_5OH]^{2+}$ | | -1501.551 | -1501.409 | -1501.392 | -1501.449 |
| $[Cr(H_2O)_4Cl_2]^{+}$ | cis | -2269.734 | -2269.628 | -2269.613 | -2269.668 |
| $[Cr(H_2O)_4Cl_2]^{+}$ | trans | -2269.736 | -2269.630 | -2269.615 | -2269.670 |
| $[Cr(H_2O)_3Cl_3]$ | mer | -2653.607 | -2653.526 | -2653.512 | -2653.567 |
| $[Cr(H_2O)_3Cl_3]$ | fac | -2653.605 | -2653.524 | -2653.510 | -2653.565 |
| α-glucopyranose-$[Cr(H_2O)_5Cl]^{2+}$ | ax1 | -2419.627 | -2419.345 | -2419.322 | -2419.397 |
| | ax2 | -2419.627 | -2419.346 | -2419.322 | -2419.399 |
| | eq1 | -2035.323 | -2035.030 | -2035.006 | -2035.081 |
| | eq2 | -2035.325 | -2035.032 | -2035.008 | -2035.083 |
| α-glucopyranose-$[Cr(H_2O)_5OH]^{2+}$ | ax1 | -2035.326 | -2035.032 | -2035.008 | -2035.083 |
| | ax2 | -2035.328 | -2035.035 | -2035.010 | -2035.086 |
| | eq1 | -2803.512 | -2803.256 | -2803.232 | -2803.307 |
| | eq2 | -2803.514 | -2803.258 | -2803.234 | -2803.310 |
| α-glucopyranose-$[Cr(H_2O)_4Cl_2]^{+}$ | ax1ax2 | -2803.509 | -2803.253 | -2803.230 | -2803.305 |
| | eq1eq2 | -2803.510 | -2803.254 | -2803.231 | -2803.306 |
| | eq1ax2 | -2803.511 | -2803.256 | -2803.232 | -2803.307 |
| | eq1ax1 | -2803.509 | -2803.254 | -2803.230 | -2803.305 |
| | eq2ax2 | -2419.627 | -2419.345 | -2419.322 | -2419.397 |
| | eq2ax1 | -2419.627 | -2419.346 | -2419.322 | -2419.399 |

**Table 24: Absolute energies of different iron(III)-complexes (PBE0/6-31+G**, CPCM(water)).**

| | non-water ligand position | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $[Fe(H_2O)_6]^{3+}$ | dublett | -1721.044 | -1720.885 | -1720.871 | -1720.922 |
| $[Fe(H_2O)_6]^{3+}$ | sextett | -1721.088 | -1720.937 | -1720.919 | -1720.979 |
| $[Fe(H_2O)_5Cl]^{2+}$ | | -2104.989 | -2104.861 | -2104.844 | -2104.904 |
| $[Fe(H_2O)_5OH]^{2+}$ | | -1720.689 | -1720.550 | -1720.532 | -1720.595 |
| $[Fe(H_2O)_4Cl_2]^{+}$ | cis | -2488.876 | -2488.772 | -2488.756 | -2488.816 |
| | trans | -2488.875 | -2488.771 | -2488.755 | -2488.813 |
| $[Fe(H_2O)_3Cl_3]$ | mer | -2872.750 | -2872.671 | -2872.657 | -2872.713 |
| | fac | -2872.755 | -2872.675 | -2872.660 | -2872.717 |
| $[Fe(H_2O)_4ClOH]^{+}$ | cis | -2104.571 | -2104.455 | -2104.439 | -2104.497 |
| | trans | -2104.568 | -2104.453 | -2104.436 | -2104.496 |
| $[Fe(H_2O)_3Cl_2OH]$ | cis | -2488.442 | -2488.352 | -2488.336 | -2488.394 |
| | trans OH | -2488.439 | -2488.348 | -2488.332 | -2488.390 |
| | trans Cl | -2488.441 | -2488.350 | -2488.335 | -2488.392 |
| $[Fe(H_2O)_2Cl_2OH_2]$ | cis | -1720.259 | -1720.132 | -1720.115 | -1720.174 |
| | trans | -1720.255 | -1720.129 | -1720.111 | -1720.172 |
| α-glucopyranose-$[Fe(H_2O)_5Cl]^{2+}$ | ax1 | -2638.764 | -2638.486 | -2638.461 | -2638.539 |
| | ax2 | -2638.766 | -2638.486 | -2638.461 | -2638.540 |
| | eq1 | -2638.766 | -2638.487 | -2638.462 | -2638.541 |
| | eq2 | -2638.768 | -2638.489 | -2638.464 | -2638.543 |
| α-glucopyranose-$[Fe(H_2O)_5OH]^{2+}$ | ax1 | -2254.465 | -2254.174 | -2254.149 | -2254.226 |
| | ax2 | -2254.467 | -2254.176 | -2254.151 | -2254.228 |
| | eq1 | -2254.466 | -2254.176 | -2254.151 | -2254.230 |
| | eq2 | -2254.467 | -2254.177 | -2254.152 | -2254.231 |
| α-glucopyranose-$[Fe(H_2O)_4Cl_2]^{+}$ | ax1ax2 | -3022.655 | -3022.401 | -3022.377 | -3022.453 |
| | eq1eq2 | -3022.659 | -3022.405 | -3022.380 | -3022.458 |
| | eq1ax2 | -3022.655 | -3022.400 | -3022.376 | -3022.454 |
| | eq1ax1 | -3022.656 | -3022.402 | -3022.378 | -3022.456 |
| | eq2ax2 | -3022.657 | -3022.402 | -3022.378 | -3022.455 |
| | eq2ax1 | -3022.654 | -3022.400 | -3022.376 | -3022.455 |

**Table 25: Absolute energies of different copper(II)-complexes (PBE0/6-31+G**, CPCM(water)).**

| | non-water ligand position | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $[Cu(H_2O)_4]^{2+}$ | quadratic-planar | -1945.203 | -1945.099 | -1945.087 | -1945.136 |
| $[Cu(H_2O)_6]^{2+}$ | | -2097.949 | -2097.796 | -2097.778 | -2097.839 |
| $[CuCl_4]^{2-}$ | tedrahedral | -3480.691 | -3480.688 | -3480.679 | -3480.725 |
| $[Cu(H_2O)Cl_3]^{-}$ | tedrahedral | -2329.089 | -2329.011 | -2329.000 | -2329.047 |
| $[Cu(H_2O)_2Cl_2]$ | quadratic planar | -2712.964 | -2712.911 | -2712.900 | -2712.947 |

**Table 26: Absolute energies of different magnesium(II)-complexes (PBE0/6-31+G**, CPCM(water)).**

| | non-water ligand position | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $[Mg(H_2O)_4]^{2+}$ | | -547.322 | -547.217 | -547.206 | -547.250 |
| $[Mg(H_2O)_6]^{2+}$ | | -658.009 | -657.860 | -657.840 | -657.904 |
| TS2 - $[MgO^1O^2(H_2O)_4]^{2+}$ | | -1191.721 | -1191.427 | -1191.400 | -1191.484 |
| | deprotonated | -1191.299 | -1191.016 | -1190.989 | -1191.070 |

**Table 27: Absolute energies for hydrogen transfer transition states with different ligand positions (PBE0/6-31+G**, CPCM(water)).**

| | | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
|---|---|---|---|---|---|
| $Al(H_2O)_6^{3+}$ | TS2 | -1386.630 | -1386.279 | -1386.249 | -1386.337 |
| | TS2 – deprot. | -1386.211 | -1385.876 | -1385.847 | -1385.932 |
| $Al(H_2O)_4^{3+}$ | TS2 | -1233.863 | -1233.562 | -1233.537 | -1233.612 |
| | TS2 – deprot. | -1233.520 | -1233.202 | -1233.179 | -1233.252 |
| $Al(H_2O)_3Cl^{2+}$ | TS2 – eq1 | -1617.761 | -1617.488 | -1617.464 | -1617.539 |
| | TS2 – ax1 - deprot | -1617.360 | -1617.097 | -1617.074 | -1617.146 |
| | TS2 – ax2 | -1617.744 | -1617.469 | -1617.445 | -1617.520 |
| | TS2 – eq2 | -1617.749 | -1617.473 | -1617.450 | -1617.525 |
| $Al(H_2O)_3OH^{2+}$ | TS2 – eq2 | -1233.458 | -1233.173 | -1233.149 | -1233.223 |
| | TS2 – ax2 | -1233.456 | -1233.171 | -1233.147 | -1233.222 |
| | TS2 – eq1 – deprot | -1233.058 | -1232.783 | -1232.759 | -1232.832 |
| | TS2 – ax1 - deprot | -1233.046 | -1232.770 | -1232.747 | -1232.820 |
| | TS2 – eq2 – deprot | -1233.058 | -1232.783 | -1232.759 | -1232.832 |
| $Al_2(H_2O)_8OH^{4+}$ | TS2 | -1780.860 | -1780.462 | -1780.428 | -1780.521 |
| | TS2 – deprot. | -1780.499 | -1780.113 | -1780.080 | -1780.170 |
| $Fe(H_2O)_4^{3+}$ | TS2 | -2254.818 | -2254.521 | -2254.495 | -2254.574 |
| | TS2 – deprot. | -2254.434 | -2254.149 | -2254.124 | -2254.202 |
| $Fe(H_2O)_3Cl^{2+}$ | TS2 – eq1 | -2638.714 | -2638.441 | -2638.416 | -2638.494 |
| | TS2 – eq1 - deprot | -2638.316 | -2638.056 | -2638.031 | -2638.109 |
| | TS2 – ax1 | -2638.715 | -2638.444 | -2638.419 | -2638.499 |
| | TS2 – ax1 - deprot | -2638.316 | -2638.056 | -2638.032 | -2638.110 |
| | TS2 – ax2 | -2638.718 | -2638.447 | -2638.422 | -2638.500 |
| | TS2 – ax2 - deprot | -2638.306 | -2638.047 | -2638.021 | -2638.103 |
| | TS2 – eq2 | -2638.713 | -2638.441 | -2638.416 | -2638.496 |
| | TS2 – eq2 - deprot | -2638.316 | -2638.056 | -2638.032 | -2638.111 |
| $Fe(H_2O)_3OH^{2+}$ | TS2 – eq2 | -2254.412 | -2254.128 | -2254.103 | -2254.183 |
| | TS2 – eq2 – deprot | -2254.005 | -2253.733 | -2253.708 | -2253.787 |
| | TS2 – ax1 - deprot | -2253.999 | -2253.728 | -2253.702 | -2253.784 |
| $Fe(H_2O)Cl_3$ | TS2 – eq1ax12 | -3406.468 | -3406.246 | -3406.222 | -3406.303 |
| | TS2 – eq12ax2 | -3406.476 | -3406.254 | -3406.230 | -3406.310 |
| $Cr(H_2O)_4^{3+}$ | TS2 | -2035.693 | -2035.394 | -2035.369 | -2035.446 |
| | TS2 – deprot. | -2035.305 | -2035.017 | -2034.993 | -2035.068 |
| $Cr(H_2O)_3OH^{2+}$ | TS2 – eq2 | -2035.274 | -2034.990 | -2034.965 | -2035.042 |
| | TS2 – eq2 – deprot | -2034.869 | -2034.595 | -2034.571 | -2034.647 |
| | TS2 – ax2 - deprot | -2034.864 | -2034.591 | -2034.566 | -2034.643 |
| $Cr(H_2O)_3Cl^{2+}$ | TS2 – eq2 | -2419.576 | -2419.304 | -2419.279 | -2419.357 |
| | TS2 – eq2 – deprot | -2419.181 | -2418.919 | -2418.895 | -2418.971 |
| | TS2 – ax2 - deprot | -2419.179 | -2418.917 | -2418.894 | -2418.969 |

**Table 28: Absolute energies forisomerization catalyzed by an $[Mg(H_2O)_6]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $[Mg(H_2O)_6]^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -1344.531 | -1344.180 | -1344.146 | -1344.244 |
| glucose | -1344.518 | -1344.169 | -1344.135 | -1344.232 |
| TS2 | -1344.468 | -1344.122 | -1344.090 | -1344.183 |
| deprot. fructose | -1344.480 | -1344.131 | -1344.099 | -1344.193 |
| fructose | -1344.521 | -1344.172 | -1344.138 | -1344.234 |
| fructofuranose O5 prot. | -1344.482 | -1344.131 | -1344.101 | -1344.185 |
| fructofuranose | -1344.537 | -1344.185 | -1344.153 | -1344.244 |

**Table 29: Absolute energies forisomerization catalyzed by an $[Mg(H_2O)_4]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $[Mg(H_2O)_4]^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -1191.786 | -1191.485 | -1191.457 | -1191.539 |
| glucose | -1191.774 | -1191.475 | -1191.447 | -1191.531 |
| TS2 | -1191.721 | -1191.427 | -1191.400 | -1191.484 |
| deprot. fructose | -1191.732 | -1191.437 | -1191.410 | -1191.495 |
| fructose | -1191.780 | -1191.482 | -1191.453 | -1191.538 |
| fructofuranose O5 prot. | -1191.323 | -1191.037 | -1191.010 | -1191.091 |
| fructofuranose | -1191.797 | -1191.495 | -1191.469 | -1191.548 |

**Table 30: Absolute energies forisomerization catalyzed by an $[Cu(H_2O)_4]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cu(H_2O)_4^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2631.720 | -2631.418 | -2631.391 | -2631.474 |
| glucose | -2631.716 | -2631.415 | -2631.388 | -2631.469 |
| deprot. glucose | -2631.286 | -2631.000 | -2630.973 | -2631.058 |
| TS2 | -2631.264 | -2630.981 | -2630.954 | -2631.037 |
| deprot. fructose | -2631.294 | -2631.008 | -2630.981 | -2631.065 |
| fructose | -2631.725 | -2631.425 | -2631.398 | -2631.481 |
| fructofuranose | -2631.726 | -2631.424 | -2631.399 | -2631.477 |

**Table 31: Absolute energies forisomerization catalyzed by an $[Cu(H_2O)_2]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cu(H_2O)_2^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2478.982 | -2478.729 | -2478.709 | -2478.777 |
| deprot. glucose | -2478.544 | -2478.307 | -2478.286 | -2478.356 |
| TS2 | -2478.520 | -2478.287 | -2478.266 | -2478.337 |
| deprot. fructose | -2478.550 | -2478.314 | -2478.292 | -2478.365 |
| fructofuranose | -2478.984 | -2478.732 | -2478.712 | -2478.779 |

**Table 32: Absolute energies forisomerization catalyzed by an $[Cu(H_2O)_6]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cu(H_2O)_6^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2784.474 | -2784.121 | -2784.088 | -2784.184 |
| glucose | -2784.465 | -2784.113 | -2784.081 | -2784.174 |
| TS2 | -2784.412 | -2784.064 | -2784.033 | -2784.126 |
| deprot. fructose | -2784.426 | -2784.078 | -2784.046 | -2784.143 |
| fructofuranose | -2784.482 | -2784.128 | -2784.097 | -2784.188 |

**Table 33: Absolute energies forisomerization catalyzed by an $[Cu(H_2O)Cl]^+$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cu(H_2O)Cl^+$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2862.870 | -2862.642 | -2862.622 | -2862.690 |
| glucose | -2862.848 | -2862.622 | -2862.602 | -2862.671 |
| TS2 | -2862.791 | -2862.570 | -2862.550 | -2862.621 |
| deprot. fructose | -2862.803 | -2862.579 | -2862.558 | -2862.631 |
| fructofuranose | -2862.869 | -2862.641 | -2862.622 | -2862.689 |

**Table 34: Absolute energies forisomerization catalyzed by an $CuCl_2$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $CuCl_2$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -3246.747 | -3246.544 | -3246.525 | -3246.593 |
| glucose | -3246.723 | -3246.523 | -3246.503 | -3246.573 |
| TS2 | -3246.669 | -3246.473 | -3246.453 | -3246.525 |
| deprot. fructose | -3246.678 | -3246.480 | -3246.459 | -3246.532 |
| fructose | -3246.733 | -3246.534 | -3246.513 | -3246.586 |
| fructofuranose | -3246.744 | -3246.542 | -3246.523 | -3246.592 |

**Table 35: Absolute energies forisomerization catalyzed by an $[Fe(H_2O)_6]^{3+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_6^{3+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2407.620 | -2407.268 | -2407.237 | -2407.329 |
| glucop. O5 prot. | -2407.608 | -2407.254 | -2407.223 | -2407.315 |
| glucose | -2407.589 | -2407.237 | -2407.205 | -2407.299 |
| TS2 | -2407.573 | -2407.226 | -2407.195 | -2407.289 |
| deprot. fructose | -2407.599 | -2407.249 | -2407.217 | -2407.311 |
| fructose | -2407.606 | -2407.256 | -2407.224 | -2407.319 |
| TS3 | -2407.597 | -2407.250 | -2407.219 | -2407.311 |
| fructofuranose O5 prot. | -2407.606 | -2407.254 | -2407.223 | -2407.314 |
| fructofuranose | -2407.632 | -2407.280 | -2407.250 | -2407.340 |

**Table 36: Absolute energies forisomerization catalyzed by an $[Fe(H_2O)_3OH]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_3OH^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2254.467 | -2254.177 | -2254.152 | -2254.232 |
| glucop. O5 prot. | -2254.447 | -2254.156 | -2254.131 | -2254.210 |
| glucose | -2254.448 | -2254.159 | -2254.134 | -2254.212 |
| TS2 | -2254.412 | -2254.128 | -2254.103 | -2254.183 |
| deprot. fructose | -2254.444 | -2254.159 | -2254.133 | -2254.214 |
| fructose | -2254.453 | -2254.165 | -2254.140 | -2254.220 |
| fructofuranose O5 prot. | -2254.453 | -2254.164 | -2254.139 | -2254.218 |
| fructofuranose | -2254.484 | -2254.195 | -2254.170 | -2254.248 |

**Table 37: Absolute energies forisomerization catalyzed by an $[Fe(H_2O)_2(OH)_2]^+$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_2(OH)_2^+$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2254.042 | -2253.766 | -2253.740 | -2253.820 |
| glucose | -2254.034 | -2253.758 | -2253.733 | -2253.812 |
| TS2 | -2253.983 | -2253.713 | -2253.687 | -2253.769 |
| deprot. fructose | -2254.005 | -2253.733 | -2253.707 | -2253.789 |
| fructofuranose | -2254.051 | -2253.774 | -2253.750 | -2253.827 |

**Table 38: Absolute energies forisomerization catalyzed by an $[Fe(H_2O)_4]^{3+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_4^{3+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2254.861 | -2254.558 | -2254.532 | -2254.610 |
| glucop. O5 prot. | -2254.859 | -2254.556 | -2254.531 | -2254.610 |
| glucose | -2254.856 | -2254.554 | -2254.529 | -2254.606 |
| deprot. glucose | -2254.466 | -2254.178 | -2254.152 | -2254.232 |
| TS2 | -2254.434 | -2254.149 | -2254.124 | -2254.202 |
| deprot. fructose | -2254.471 | -2254.184 | -2254.157 | -2254.239 |
| fructose | -2254.866 | -2254.566 | -2254.540 | -2254.620 |
| TS3 | -2254.855 | -2254.554 | -2254.529 | -2254.607 |
| fructofuranose O5 prot. | -2254.859 | -2254.532 | -2254.531 | -2254.611 |
| fructofuranose | -2254.887 | -2254.586 | -2254.561 | -2254.639 |

**Table 39: Absolute energies forisomerization catalyzed by an $[Fe_2(H_2O)_8(OH)_2]^{4+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe_2(H_2O)_8(OH)_2^{4+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2254.861 | -2254.558 | -2254.532 | -2254.610 |
| deprot. glucose | -3822.411 | -3822.026 | -3821.992 | -3822.089 |
| TS2 | -3822.389 | -3822.011 | -3821.975 | -3822.076 |
| deprot. fructose | -3822.436 | -3822.054 | -3822.018 | -3822.121 |

**Table 40: Absolute energies forisomerization catalyzed by an $[Fe(H_2O)_3Cl]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_3Cl^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2638.768 | -2638.489 | -2638.464 | -2638.544 |
| glucop. O5 prot. | -2638.752 | -2638.473 | -2638.448 | -2638.526 |
| glucose | -2638.756 | -2638.479 | -2638.454 | -2638.532 |
| TS2 | -2638.713 | -2638.441 | -2638.416 | -2638.496 |
| deprot. fructose | -2638.731 | -2638.455 | -2638.430 | -2638.510 |
| fructose | -2638.767 | -2638.491 | -2638.466 | -2638.547 |
| fructofuranose O5 prot. | -2638.760 | -2638.482 | -2638.457 | -2638.534 |
| fructofuranose | -2638.788 | -2638.510 | -2638.485 | -2638.561 |

**Table 41: Absolute energies forisomerization catalyzed by an $[Fe(H_2O)_2(OH)Cl]^+$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_2(OH)Cl^+$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2638.353 | -2638.087 | -2638.062 | -2638.142 |
| glucose | -2638.340 | -2638.075 | -2638.051 | -2638.129 |
| TS2 | -2638.294 | -2638.036 | -2638.010 | -2638.092 |
| deprot. fructose | -2638.316 | -2638.057 | -2638.031 | -2638.114 |
| fructofuranose | -2638.363 | -2638.097 | -2638.073 | -2638.150 |

**Table 42: Absolute energies forisomerization catalyzed by an $[Fe(H_2O)_2Cl_2]^+$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)_2Cl_2^+$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -3022.659 | -3022.405 | -3022.380 | -3022.458 |
| glucop. O5 prot. | -3022.634 | -3022.379 | -3022.355 | -3022.432 |
| glucose | -3022.642 | -3022.390 | -3022.365 | -3022.444 |
| TS2 | -3022.590 | -3022.344 | -3022.318 | -3022.402 |
| deprot. fructose | -3022.630 | -3022.382 | -3022.356 | -3022.440 |
| fructose | -3022.636 | -3022.385 | -3022.359 | -3022.442 |
| fructofuranose O5 prot. | -3022.638 | -3022.385 | -3022.361 | -3022.439 |
| fructofuranose | -3022.667 | -3022.413 | -3022.389 | -3022.466 |

**Table 43: Absolute energies forisomerization catalyzed by an $Fe(H_2O)(OH)Cl_2$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)(OH)Cl_2$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -3022.225 | -3021.985 | -3021.960 | -3022.038 |
| glucose | -3022.210 | -3021.971 | -3021.947 | -3022.026 |
| TS2 | -3022.167 | -3021.933 | -3021.909 | -3021.988 |
| deprot. fructose | -3022.188 | -3021.952 | -3021.927 | -3022.008 |
| fructofuranose | -3022.228 | -3021.987 | -3021.963 | -3022.041 |

**Table 44: Absolute energies forisomerization catalyzed by an $[Fe(OH)Cl_3]^-$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(OH)Cl_3^-$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| TS2 | -3406.025 | -3405.816 | -3405.792 | -3405.872 |

**Table 45: Absolute energies forisomerization catalyzed by an $Fe(H_2O)Cl_3$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Fe(H_2O)Cl_3$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -3406.529 | -3406.300 | -3406.276 | -3406.354 |
| glucose | -3406.516 | -3406.289 | -3406.265 | -3406.344 |
| TS2 | -3406.468 | -3406.246 | -3406.222 | -3406.303 |
| deprot. fructose | -3406.499 | -3406.274 | -3406.250 | -3406.330 |
| fructofuranose | -3406.527 | -3406.299 | -3406.275 | -3406.354 |

**Table 46: Absolute energies forisomerization catalyzed by an $[Cr(H_2O)_4]^{3+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)_4^{3+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2035.731 | -2035.424 | -2035.400 | -2035.475 |
| glucop. O5 prot. | -2035.724 | -2035.418 | -2035.394 | -2035.469 |
| glucose | -2035.73 | -2035.424 | -2035.400 | -2035.475 |
| deprot. glucose | -2035.329 | -2035.038 | -2035.014 | -2035.090 |
| TS2 | -2035.305 | -2035.017 | -2034.993 | -2035.068 |
| deprot. fructose | -2035.335 | -2035.045 | -2035.020 | -2035.097 |
| fructose | -2035.736 | -2035.432 | -2035.408 | -2035.484 |
| TS3 | -2035.724 | -2035.420 | -2035.396 | -2035.472 |
| fructofuranose O5 prot. | -2035.735 | -2035.430 | -2035.406 | -2035.481 |
| fructofuranose | -2035.758 | -2035.453 | -2035.430 | -2035.503 |

**Table 47: Absolute energies forisomerization catalyzed by an $[r_2(H_2O)_8(OH)_2]^{4+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr_2(H_2O)_8(OH)_2^{4+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| deprot. glucose | -3384.127 | -3383.740 | -3383.706 | -3383.800 |
| TS2 | -3384.117 | -3383.733 | -3383.700 | -3383.794 |
| deprot. fructose | -3384.168 | -3383.781 | -3383.747 | -3383.842 |

**Table 48: Absolute energies forisomerization catalyzed by an $Cr(H_2O)_6^{3+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)_6^{3+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2188.492 | -2188.135 | -2188.106 | -2188.192 |
| glucop. O5 prot. | -2188.474 | -2188.089 | -2188.088 | -2188.176 |
| TS1 | -2188.469 | -2188.117 | -2188.088 | -2188.173 |
| glucose | -2188.484 | -2188.130 | -2188.100 | -2188.189 |
| TS2 | -2188.440 | -2188.090 | -2188.060 | -2188.149 |
| deprot. fructose | -2188.466 | -2188.112 | -2188.083 | -2188.170 |
| fructose | -2188.479 | -2188.123 | -2188.094 | -2188.181 |
| TS3 | -2188.473 | -2188.118 | -2188.090 | -2188.174 |
| fructofuranose O5 prot. | -2188.473 | -2188.118 | -2188.090 | -2188.174 |
| fructofuranose | -2188.504 | -2188.148 | -2188.119 | -2188.203 |

**Table 49: Absolute energies forisomerization catalyzed by an $[Cr(H_2O)_3OH]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)_3OH^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2035.329 | -2035.036 | -2035.011 | -2035.087 |
| glucop. O5 prot. | -2035.306 | -2035.013 | -2034.989 | -2035.064 |
| glucose | -2035.325 | -2035.035 | -2035.010 | -2035.086 |
| TS2 | -2035.274 | -2034.990 | -2034.965 | -2035.042 |
| deprot. fructose | -2035.297 | -2035.009 | -2034.984 | -2035.064 |
| fructose | -2035.317 | -2035.028 | -2035.002 | -2035.084 |
| TS3 | -2035.311 | -2035.020 | -2034.996 | -2035.071 |
| fructofuranose O5 prot. | -2035.313 | -2035.022 | -2034.998 | -2035.074 |
| fructofuranose | -2035.346 | -2035.054 | -2035.031 | -2035.104 |

**Table 50: Absolute energies forisomerization catalyzed by an $[Cr(H_2O)_3Cl]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)_3Cl^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2419.628 | -2419.347 | -2419.323 | -2419.398 |
| glucop. O5 prot. | -2419.609 | -2419.328 | -2419.304 | -2419.378 |
| glucose | -2419.617 | -2419.338 | -2419.314 | -2419.390 |
| TS2 | -2419.576 | -2419.304 | -2419.279 | -2419.357 |
| deprot. fructose | -2419.601 | -2419.325 | -2419.299 | -2419.379 |
| fructose | -2419.628 | -2419.350 | -2419.325 | -2419.402 |
| TS3 | -2419.614 | -2419.335 | -2419.311 | -2419.387 |
| fructofuranose O5 prot. | -2419.622 | -2419.341 | -2419.318 | -2419.392 |
| fructofuranose | -2419.650 | -2419.370 | -2419.347 | -2419.420 |

**Table 51: Absolute energies forisomerization catalyzed by an $[Cr(H_2O)_2Cl_2]^{+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)_2Cl_2^{+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -2803.514 | -2803.258 | -2803.234 | -2803.310 |
| glucop. O5 prot. | -2803.488 | -2803.232 | -2803.209 | -2803.284 |
| glucose | -2803.497 | -2803.244 | -2803.220 | -2803.298 |
| TS2 | -2803.450 | -2803.204 | -2803.180 | -2803.258 |
| deprot. fructose | -2803.473 | -2803.222 | -2803.198 | -2803.276 |
| fructose | -2803.505 | -2803.252 | -2803.228 | -2803.304 |
| fructofuranose O5 prot. | -2803.495 | -2803.240 | -2803.217 | -2803.292 |
| fructofuranose | -2803.529 | -2803.273 | -2803.250 | -2803.322 |

**Table 52: Absolute energies forisomerization catalyzed by an $Cr(H_2O)Cl_3$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Cr(H_2O)Cl_3$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -3187.382 | -3187.151 | -3187.128 | -3187.203 |
| glucose | -3187.372 | -3187.143 | -3187.120 | -3187.197 |
| TS2 | -3187.321 | -3187.099 | -3187.076 | -3187.152 |
| deprot. fructose | -3187.336 | -3187.110 | -3187.086 | -3187.164 |
| fructofuranose | -3187.389 | -3187.159 | -3187.137 | -3187.210 |

**Table 53: Absolute energies forisomerization catalyzed by an $[Al(H_2O)_6]^{3+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Al(H_2O)_6^{3+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -1386.685 | -1386.327 | -1386.298 | -1386.384 |
| glucop. O5 prot. | -1386.664 | -1386.307 | -1386.277 | -1386.363 |
| TS1 | -1386.660 | -1386.308 | -1386.278 | -1386.363 |
| glucose | -1386.677 | -1386.320 | -1386.291 | -1386.376 |
| TS2 | -1386.630 | -1386.279 | -1386.249 | -1386.337 |
| deprot. fructose | -1386.653 | -1386.298 | -1386.269 | -1386.354 |
| fructose | -1386.669 | -1386.315 | -1386.284 | -1386.372 |
| TS3 | -1386.659 | -1386.307 | -1386.278 | -1386.362 |
| fructofuranose O5 prot. | -1386.663 | -1386.306 | -1386.277 | -1386.361 |
| fructofuranose | -1386.688 | -1386.332 | -1386.303 | -1386.389 |

**Table 54: Absolute energies forisomerization catalyzed by an $[Al(H_2O)_3OH]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Al(H_2O)_3OH^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -1233.512 | -1233.218 | -1233.194 | -1233.267 |
| glucop. O5 prot. | -1233.491 | -1233.196 | -1233.173 | -1233.245 |
| glucose | -1233.499 | -1233.209 | -1233.185 | -1233.258 |
| TS2 | -1233.458 | -1233.173 | -1233.149 | -1233.223 |
| deprot. fructose | -1233.482 | -1233.192 | -1233.167 | -1233.242 |
| fructose | -1233.514 | -1233.223 | -1233.198 | -1233.273 |
| TS3 | -1233.502 | -1233.211 | -1233.187 | -1233.260 |
| fructofuranose O5 prot. | -1233.507 | -1233.214 | -1233.190 | -1233.262 |
| fructofuranose | -1233.535 | -1233.241 | -1233.218 | -1233.289 |

**Table 55: Absolute energies forisomerization catalyzed by an $[Al(H_2O)_3Cl]^{2+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Al(H_2O)_3Cl^{2+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -1617.809 | -1617.526 | -1617.503 | -1617.575 |
| glucop. O5 prot. | -1617.794 | -1617.512 | -1617.488 | -1617.561 |
| glucose | -1617.800 | -1617.521 | -1617.497 | -1617.571 |
| TS2 | -1617.761 | -1617.488 | -1617.464 | -1617.539 |
| deprot. fructose | -1617.787 | -1617.510 | -1617.486 | -1617.562 |
| fructose | -1617.800 | -1617.522 | -1617.497 | -1617.574 |
| TS3 | -1617.794 | -1617.514 | -1617.490 | -1617.564 |
| fructofuranose O5 prot. | -1617.800 | -1617.518 | -1617.495 | -1617.568 |
| fructofuranose | -1617.828 | -1617.546 | -1617.524 | -1617.594 |

**Table 56: Absolute energies forisomerization catalyzed by an $[Al(H_2O)_4]^{3+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Al(H_2O)_4^{3+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -1233.920 | -1233.614 | -1233.589 | -1233.664 |
| glucop. O5 prot. | -1233.907 | -1233.601 | -1233.576 | -1233.650 |
| glucose | -1233.913 | -1233.608 | -1233.584 | -1233.656 |
| deprot. glucose | -1233.515 | -1233.223 | -1233.199 | -1233.272 |
| TS2 | -1233.520 | -1233.202 | -1233.179 | -1233.252 |
| deprot. fructose | -1233.520 | -1233.228 | -1233.204 | -1233.278 |
| fructose | -1233.924 | -1233.620 | -1233.595 | -1233.670 |
| TS3 | -1233.914 | -1233.584 | -1233.584 | -1233.656 |
| fructofuranose O5 prot. | -1233.923 | -1233.617 | -1233.593 | -1233.666 |
| fructofuranose | -1233.948 | -1233.642 | -1233.619 | -1233.690 |

**Table 57: Absolute energies forisomerization catalyzed by an $[Al_2(H_2O)_8(OH)_2]^{4+}$ complex (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $Al_2(H_2O)_8(OH)_2^{4+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| compl. gluc. | -1233.920 | -1233.614 | -1233.589 | -1233.664 |
| deprot. glucose | -1780.508 | -1780.119 | -1780.086 | -1780.177 |
| TS2 | -1780.499 | -1780.113 | -1780.080 | -1780.170 |
| deprot. fructose | -1780.548 | -1780.159 | -1780.125 | -1780.218 |

**Table 58: Absolute energies for the keto-enol-tautomerization mechanism (PBE0/6-31+G**, CPCM(water)).**

| catalyst → | $[Al(H_2O)_4]^{3+}$ | | | |
|---|---|---|---|---|
| structure ↓ | E / a.u. | E_ZPC / a.u. | H / a.u. | G / a.u. |
| A | -1233.913 | -1233.608 | -1233.584 | -1233.656 |
| B | -1233.500 | -1233.207 | -1233.184 | -1233.256 |
| C | -1233.896 | -1233.591 | -1233.567 | -1233.640 |
| D | -1233.503 | -1233.211 | -1233.186 | -1233.260 |
| E | -1233.926 | -1233.622 | -1233.597 | -1233.672 |

# Coordinates of important structures

Cartesian coordinates are given for important structures like every catalyst-glucopyranose, catalyst-fructofuranose and hydrogen transfer transition state TS2 for the lowest reaction pathways discussed in the Result section.

$[Mg(H_2O)_4]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.053 | 0.789 | 4.533 |
| 6 | -1.048 | 0.528 | 3.411 |
| 6 | -0.409 | -0.295 | 2.310 |
| 6 | 0.920 | 0.297 | 1.856 |
| 8 | 1.745 | 0.613 | 2.917 |
| 6 | 1.189 | 1.459 | 3.937 |
| 8 | -2.180 | -0.194 | 3.844 |
| 8 | -1.257 | -0.352 | 1.158 |
| 12 | -1.042 | 1.155 | -0.287 |
| 8 | -0.571 | 2.692 | -1.594 |
| 8 | 0.590 | 1.446 | 1.062 |
| 6 | 2.279 | 1.690 | 4.956 |
| 8 | 3.276 | 2.507 | 4.370 |
| 8 | -0.710 | 1.636 | 5.457 |
| 8 | 0.083 | -0.198 | -1.402 |
| 8 | -2.679 | 0.618 | -1.431 |
| 8 | -2.234 | 2.534 | 0.726 |
| 1 | 3.971 | 2.655 | 5.021 |
| 1 | 0.903 | 2.424 | 3.497 |
| 1 | 2.691 | 0.721 | 5.269 |
| 1 | 1.834 | 2.181 | 5.830 |
| 1 | -0.470 | 1.388 | 6.355 |
| 1 | 0.227 | -0.164 | 5.003 |
| 1 | -1.351 | 1.504 | 3.003 |
| 1 | 1.478 | -0.414 | 1.240 |
| 1 | -0.228 | -1.313 | 2.671 |
| 1 | -2.630 | 0.337 | 4.513 |
| 1 | -2.109 | -0.737 | 1.408 |
| 1 | -3.073 | 2.361 | 1.170 |
| 1 | -2.266 | 3.446 | 0.412 |
| 1 | -1.089 | 2.804 | -2.400 |
| 1 | 0.268 | 3.146 | -1.733 |
| 1 | 0.485 | -0.012 | -2.259 |
| 1 | 0.051 | -1.157 | -1.303 |
| 1 | -3.595 | 0.882 | -1.288 |
| 1 | -2.687 | -0.137 | -2.030 |
| 1 | 1.414 | 1.842 | 0.742 |

$[Mg(H_2O)_4]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.048 | 0.837 | 1.028 |
| 6 | 0.956 | 0.404 | 1.837 |
| 6 | 0.509 | -1.023 | 2.017 |
| 6 | 0.451 | -1.386 | 3.542 |
| 6 | -0.932 | -1.116 | 4.138 |
| 8 | -1.427 | 0.144 | 3.666 |
| 8 | 2.380 | 2.095 | 1.014 |
| 12 | 1.338 | 3.360 | 2.162 |
| 8 | -0.085 | 4.331 | 3.306 |
| 8 | 2.255 | 3.042 | 4.034 |
| 8 | 2.728 | 4.902 | 1.983 |
| 8 | 0.163 | 3.878 | 0.508 |
| 8 | 0.300 | 1.372 | 2.432 |
| 8 | 1.409 | -1.842 | 1.334 |
| 8 | 0.686 | -2.774 | 3.642 |
| 6 | -0.923 | -1.097 | 5.655 |
| 8 | -2.220 | -0.660 | 6.032 |
| 1 | -2.207 | -0.367 | 6.950 |
| 1 | -1.610 | -1.900 | 3.778 |
| 1 | -0.158 | -0.397 | 6.015 |
| 1 | -0.704 | -2.099 | 6.039 |
| 1 | 1.471 | -2.936 | 4.177 |
| 1 | 1.225 | -0.827 | 4.081 |
| 1 | -0.506 | -1.126 | 1.600 |
| 1 | 2.734 | 0.061 | 0.675 |
| 1 | 1.044 | 0.555 | 0.335 |
| 1 | 1.371 | -2.706 | 1.778 |
| 1 | 2.246 | 2.218 | 4.535 |
| 1 | 3.128 | 3.435 | 4.156 |
| 1 | 2.492 | 5.834 | 2.067 |
| 1 | 3.390 | 4.847 | 1.284 |
| 1 | -0.238 | 4.742 | 0.358 |
| 1 | 0.511 | 3.585 | -0.343 |
| 1 | 0.005 | 4.332 | 4.267 |
| 1 | -1.015 | 4.484 | 3.103 |
| 1 | -2.054 | 0.477 | 4.332 |
| 1 | -0.509 | 1.003 | 2.975 |

$[Mg(H_2O)_4]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -2.094 | -1.710 | 1.464 |
| 6 | -2.779 | -0.798 | 2.329 |
| 6 | -2.432 | 0.631 | 1.960 |
| 6 | -2.785 | 1.023 | 0.518 |
| 6 | -1.485 | 1.650 | 0.006 |
| 6 | -0.420 | 0.922 | 0.837 |
| 8 | -1.004 | 0.815 | 2.093 |
| 6 | 0.934 | 1.606 | 0.995 |
| 8 | 1.754 | 1.342 | -0.146 |
| 12 | 1.620 | -0.692 | -0.771 |
| 8 | -3.890 | 1.897 | 0.532 |
| 8 | -1.260 | 1.507 | -1.381 |
| 8 | -0.142 | -0.370 | 0.291 |
| 8 | 0.551 | -0.188 | -2.471 |
| 8 | 1.335 | -2.658 | -1.332 |
| 8 | 2.582 | -1.281 | 0.978 |
| 8 | 3.495 | -0.612 | -1.651 |
| 1 | -2.724 | -2.242 | 0.965 |
| 1 | -3.862 | -0.940 | 2.265 |
| 1 | -2.459 | -0.999 | 3.356 |
| 1 | -4.316 | 1.883 | -0.333 |
| 1 | -1.651 | 2.248 | -1.858 |
| 1 | -0.182 | 0.423 | -2.238 |
| 1 | -1.474 | 2.709 | 0.289 |
| 1 | 0.822 | 2.680 | 1.151 |
| 1 | 1.628 | 2.028 | -0.813 |
| 1 | 1.440 | 1.166 | 1.857 |
| 1 | -0.822 | -1.012 | 0.628 |
| 1 | 0.678 | -2.887 | -2.001 |
| 1 | 1.463 | -3.432 | -0.773 |
| 1 | 3.777 | -1.241 | -2.326 |
| 1 | 3.510 | -1.544 | 0.976 |
| 1 | 2.162 | -1.715 | 1.729 |
| 1 | 4.010 | 0.193 | -1.783 |
| 1 | -3.005 | 0.134 | -0.088 |
| 1 | -2.920 | 1.317 | 2.658 |
| 1 | 0.953 | 0.130 | -3.287 |

$[Mg(H_2O)_6]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.512 | -1.968 | 1.082 |
| 6 | 0.317 | -1.174 | 2.097 |
| 8 | -0.493 | -0.766 | 3.162 |
| 6 | -1.603 | 0.060 | 2.801 |
| 6 | -2.525 | -0.714 | 1.863 |
| 6 | -1.746 | -1.193 | 0.647 |
| 8 | 0.938 | -0.084 | 1.450 |
| 6 | -2.300 | 0.469 | 4.078 |
| 8 | -1.464 | 1.376 | 4.777 |
| 8 | -3.587 | 0.131 | 1.472 |
| 8 | -2.630 | -1.995 | -0.110 |
| 8 | 0.222 | -2.317 | -0.082 |
| 8 | 0.789 | 1.483 | -0.748 |
| 12 | 1.670 | 0.884 | -2.517 |
| 8 | 2.611 | 0.446 | -4.330 |
| 8 | 2.407 | 2.823 | -2.729 |
| 8 | 0.905 | -1.021 | -2.358 |

| | | | |
|---|---|---|---|
| 8 | 0.030 | 1.457 | -3.679 |
| 8 | 3.434 | 0.280 | -1.572 |
| 1 | -1.913 | 1.639 | 5.587 |
| 1 | -2.501 | -0.429 | 4.679 |
| 1 | -3.256 | 0.935 | 3.812 |
| 1 | -1.241 | 0.964 | 2.292 |
| 1 | -2.913 | -1.598 | 2.395 |
| 1 | -4.086 | -0.336 | 0.789 |
| 1 | -1.445 | -0.312 | 0.061 |
| 1 | -2.216 | -2.206 | -0.955 |
| 1 | -0.845 | -2.881 | 1.590 |
| 1 | 0.772 | -3.091 | 0.090 |
| 1 | 1.082 | -1.815 | 2.547 |
| 1 | 4.035 | 0.902 | -1.145 |
| 1 | 0.012 | 2.052 | -0.725 |
| 1 | 2.481 | 3.456 | -2.005 |
| 1 | -0.169 | 2.380 | -3.876 |
| 1 | 3.412 | -0.086 | -4.404 |
| 1 | 0.648 | -1.471 | -1.521 |
| 1 | -0.810 | 0.984 | -3.649 |
| 1 | 1.095 | -1.706 | -3.008 |
| 1 | 2.130 | 0.365 | -5.161 |
| 1 | 3.495 | -0.549 | -1.083 |
| 1 | 0.778 | 0.930 | 0.063 |
| 1 | 3.070 | 3.059 | -3.387 |
| 1 | 1.592 | 0.300 | 2.048 |

$[Mg(H_2O)_6]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | -0.383 | -0.833 | 2.328 |
| 6 | -0.273 | -1.451 | 3.614 |
| 8 | 0.534 | -2.460 | 3.780 |
| 8 | 0.191 | -1.276 | 1.250 |
| 6 | -1.070 | -0.949 | 4.805 |
| 8 | -2.106 | -1.896 | 4.918 |
| 6 | -0.202 | -0.828 | 6.070 |
| 8 | 0.402 | -2.111 | 6.283 |
| 6 | -1.016 | -0.357 | 7.272 |
| 6 | -0.197 | -0.208 | 8.548 |
| 8 | -1.062 | 0.103 | 9.628 |
| 8 | -2.072 | -1.279 | 7.494 |
| 8 | 2.195 | -2.805 | 0.767 |
| 12 | 1.199 | -4.499 | 0.131 |
| 8 | 2.767 | -5.831 | 0.506 |
| 8 | -0.472 | -3.310 | -0.218 |
| 8 | 0.599 | -4.856 | 2.108 |
| 8 | 2.051 | -4.264 | -1.766 |
| 8 | 0.135 | -6.135 | -0.604 |
| 1 | -1.431 | 0.629 | 7.005 |
| 1 | -1.242 | -0.150 | 2.246 |
| 1 | -1.276 | 1.043 | 9.601 |
| 1 | 0.584 | 0.551 | 8.420 |
| 1 | 0.272 | -1.161 | 8.807 |
| 1 | 1.213 | -2.019 | 6.798 |
| 1 | 0.572 | -0.075 | 5.874 |
| 1 | -1.457 | 0.053 | 4.571 |
| 1 | 0.652 | -2.591 | 4.773 |
| 1 | -2.490 | -1.043 | 8.335 |
| 1 | -2.442 | -1.846 | 5.834 |
| 1 | 2.411 | -3.410 | -2.030 |
| 1 | 1.665 | -4.665 | -2.554 |
| 1 | 0.451 | -7.040 | -0.498 |
| 1 | -0.827 | -6.171 | -0.661 |
| 1 | 3.567 | -5.839 | -0.031 |
| 1 | -0.414 | -2.462 | 0.307 |
| 1 | 3.022 | -6.065 | 1.406 |
| 1 | -0.738 | -3.075 | -1.114 |
| 1 | 0.544 | -4.092 | 2.705 |
| 1 | 2.958 | -2.823 | 1.354 |
| 1 | 1.552 | -2.108 | 1.097 |
| 1 | -0.158 | -5.419 | 2.308 |
| 1 | 0.348 | -0.150 | 3.053 |

$[Mg(H_2O)_6]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.158 | 0.747 | -3.850 |
| 6 | 0.982 | 1.563 | -3.865 |
| 6 | 1.175 | 1.861 | -5.360 |
| 6 | 0.784 | 0.550 | -6.034 |
| 6 | -0.206 | -0.077 | -5.032 |
| 6 | 0.656 | 2.751 | -2.978 |
| 8 | 1.778 | 3.616 | -2.880 |
| 8 | 2.096 | 0.888 | -3.324 |
| 8 | 2.486 | 2.300 | -5.645 |
| 8 | 0.224 | 0.827 | -7.300 |
| 6 | 0.107 | -1.513 | -4.665 |
| 8 | 1.463 | -1.575 | -4.227 |
| 8 | 4.333 | 3.932 | -3.696 |
| 12 | 5.672 | 2.389 | -3.324 |
| 8 | 6.590 | 3.290 | -1.662 |
| 8 | 4.903 | 1.274 | -4.909 |
| 8 | 4.278 | 1.632 | -1.992 |
| 8 | 7.215 | 3.284 | -4.434 |
| 8 | 7.067 | 0.840 | -3.051 |
| 1 | 1.620 | -2.404 | -3.761 |
| 1 | -0.572 | -1.840 | -3.870 |
| 1 | -0.039 | -2.153 | -5.544 |
| 1 | -1.223 | -0.023 | -5.433 |
| 1 | 1.678 | -0.076 | -6.140 |
| 1 | -0.204 | 3.278 | -3.405 |
| 1 | 3.393 | 3.773 | -3.451 |
| 1 | 4.305 | 4.353 | -4.563 |
| 1 | 0.448 | 2.629 | -5.655 |
| 1 | 2.511 | 2.637 | -6.550 |
| 1 | 0.262 | 0.033 | -7.845 |
| 1 | 5.416 | 1.148 | -5.714 |
| 1 | 3.992 | 1.523 | -5.188 |
| 1 | 2.026 | -0.066 | -3.564 |
| 1 | 7.220 | 4.005 | -1.811 |
| 1 | 6.069 | 3.532 | -0.888 |
| 1 | 4.528 | 0.945 | -1.365 |
| 1 | 7.584 | 0.796 | -2.237 |
| 1 | 6.885 | -0.068 | -3.319 |
| 1 | 3.412 | 1.365 | -2.386 |
| 1 | 7.963 | 2.728 | -4.685 |
| 1 | 7.161 | 3.993 | -5.085 |
| 1 | 0.384 | 2.360 | -1.991 |
| 1 | 1.584 | 4.303 | -2.233 |

$[Cu(H_2O)_4]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.717 | -0.532 | 1.977 |
| 6 | -0.189 | -1.188 | 0.718 |
| 6 | 1.100 | -0.548 | 0.189 |
| 8 | 2.006 | -0.217 | 1.157 |
| 6 | 1.532 | 0.473 | 2.330 |
| 6 | 0.412 | -0.339 | 2.983 |
| 8 | -1.156 | -1.097 | -0.340 |
| 29 | -0.726 | 0.112 | -1.888 |
| 8 | 0.406 | -1.572 | -2.965 |
| 8 | 0.755 | 0.595 | -0.658 |
| 6 | 2.731 | 0.667 | 3.226 |
| 8 | 3.600 | 1.598 | 2.612 |
| 8 | -0.154 | 0.348 | 4.081 |
| 8 | -1.737 | -1.356 | 2.486 |
| 8 | -2.226 | -0.592 | -2.950 |
| 8 | -2.260 | 1.669 | -1.298 |
| 8 | -0.093 | 1.483 | -3.204 |
| 1 | 4.361 | 1.731 | 3.186 |
| 1 | 1.149 | 1.467 | 2.054 |
| 1 | 3.224 | -0.303 | 3.378 |
| 1 | 2.377 | 1.038 | 4.196 |
| 1 | 0.214 | 0.010 | 4.904 |
| 1 | 0.800 | -1.321 | 3.289 |
| 1 | -1.121 | 0.463 | 1.735 |
| 1 | 1.599 | -1.223 | -0.507 |
| 1 | 0.018 | -2.243 | 0.923 |
| 1 | -2.042 | -0.957 | 3.312 |
| 1 | -1.664 | -1.912 | -0.447 |
| 1 | -2.742 | 1.659 | -0.462 |
| 1 | -2.072 | 2.595 | -1.491 |
| 1 | -0.393 | 1.425 | -4.121 |
| 1 | 0.861 | 1.636 | -3.231 |
| 1 | 1.212 | -1.441 | -3.478 |
| 1 | 0.390 | -2.506 | -2.723 |
| 1 | -2.941 | 0.037 | -3.120 |
| 1 | -1.997 | -1.033 | -3.781 |
| 1 | 0.580 | 1.392 | -0.134 |

$[Cu(H_2O)_4]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.061 | 0.692 | 0.810 |
| 6 | 0.908 | 0.394 | 1.596 |
| 6 | 0.589 | -0.990 | 2.123 |
| 6 | 0.845 | -0.993 | 3.656 |
| 6 | -0.364 | -0.467 | 4.428 |
| 8 | 0.099 | 0.076 | 5.668 |
| 8 | 2.346 | 1.937 | 0.595 |
| 29 | 1.170 | 3.036 | 1.669 |
| 8 | 0.379 | 4.046 | 3.194 |
| 8 | 0.225 | 1.404 | 2.051 |
| 8 | 2.283 | 4.655 | 1.261 |
| 8 | -0.542 | 3.969 | 0.445 |
| 8 | 1.402 | -1.929 | 1.472 |
| 8 | 1.174 | -2.329 | 4.002 |
| 6 | -1.413 | -1.526 | 4.713 |
| 8 | -2.396 | -0.883 | 5.516 |
| 8 | 0.751 | 2.752 | 5.424 |
| 1 | -2.924 | -1.552 | 5.964 |
| 1 | -0.819 | 0.340 | 3.839 |
| 1 | -0.959 | -2.365 | 5.251 |
| 1 | -1.846 | -1.898 | 3.777 |
| 1 | 1.856 | -2.328 | 4.683 |
| 1 | 1.696 | -0.336 | 3.873 |
| 1 | -0.473 | -1.203 | 1.930 |
| 1 | 2.723 | -0.102 | 0.462 |
| 1 | 0.881 | 0.257 | 0.250 |
| 1 | 1.618 | -2.597 | 2.144 |
| 1 | 0.522 | 1.800 | 5.515 |
| 1 | 0.444 | 3.184 | 6.228 |
| 1 | 2.346 | 5.265 | 2.008 |
| 1 | 3.186 | 4.450 | 0.984 |
| 1 | -0.280 | 4.630 | -0.207 |
| 1 | -1.099 | 3.340 | -0.028 |
| 1 | 0.439 | 3.540 | 4.058 |
| 1 | -0.551 | 4.239 | 3.023 |
| 1 | -0.670 | 0.062 | 6.262 |

$[Cu(H_2O)_4]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.876 | -0.430 | -0.112 |
| 6 | -1.141 | -0.325 | -1.497 |

| | | | |
|---|---|---|---|
| 6 | -0.469 | 0.917 | -2.020 |
| 6 | -0.801 | 1.256 | -3.470 |
| 6 | 0.485 | 1.951 | -3.915 |
| 6 | 1.552 | 1.138 | -3.179 |
| 8 | 0.977 | 0.770 | -1.984 |
| 6 | 2.903 | 1.789 | -2.911 |
| 8 | 3.729 | 1.726 | -4.077 |
| 29 | 3.509 | -0.166 | -4.983 |
| 8 | -1.943 | 2.072 | -3.516 |
| 8 | 0.694 | 1.998 | -5.306 |
| 8 | 1.818 | -0.085 | -3.962 |
| 8 | 2.369 | 0.417 | -6.734 |
| 8 | 3.193 | -2.065 | -5.825 |
| 8 | 4.539 | -0.941 | -3.178 |
| 8 | 5.146 | -0.083 | -6.050 |
| 1 | -1.302 | -1.226 | 0.224 |
| 1 | -0.772 | -1.204 | -2.042 |
| 1 | -2.218 | -0.225 | -1.693 |
| 1 | -2.356 | 1.991 | -4.382 |
| 1 | 0.354 | 2.828 | -5.660 |
| 1 | 1.659 | 1.005 | -6.403 |
| 1 | 0.491 | 2.964 | -3.494 |
| 1 | 2.780 | 2.823 | -2.583 |
| 1 | 3.570 | 2.488 | -4.650 |
| 1 | 3.412 | 1.218 | -2.133 |
| 1 | 1.721 | -0.827 | -3.343 |
| 1 | 2.508 | -1.984 | -6.503 |
| 1 | 2.991 | -2.858 | -5.313 |
| 1 | 5.486 | -0.956 | -6.293 |
| 1 | 5.430 | -0.621 | -2.988 |
| 1 | 4.554 | -1.885 | -2.981 |
| 1 | 5.892 | 0.433 | -5.715 |
| 1 | -0.941 | 0.343 | -4.065 |
| 1 | -0.725 | 1.770 | -1.380 |
| 1 | 2.849 | 0.905 | -7.413 |

$[CuCl_2]$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.044 | 0.768 | 4.560 |
| 6 | -1.032 | 0.421 | 3.440 |
| 6 | -0.308 | -0.411 | 2.391 |
| 6 | 0.312 | -1.640 | 3.025 |
| 6 | 1.155 | -1.282 | 4.243 |
| 8 | 0.500 | -0.441 | 5.115 |
| 8 | -1.492 | 1.584 | 2.777 |
| 8 | -1.164 | -0.877 | 1.373 |
| 8 | 1.189 | -2.309 | 2.113 |
| 29 | 3.073 | -1.567 | 2.008 |
| 8 | 2.346 | -0.685 | 3.700 |
| 6 | -0.687 | 1.522 | 5.699 |
| 8 | 0.334 | 1.994 | 6.559 |
| 17 | 5.118 | -0.903 | 2.486 |
| 17 | 3.328 | -2.356 | -0.033 |
| 1 | -0.078 | 2.465 | 7.292 |
| 1 | 0.771 | 1.377 | 4.145 |
| 1 | -1.377 | 0.852 | 6.230 |
| 1 | -1.263 | 2.356 | 5.279 |
| 1 | -2.370 | 1.815 | 3.096 |
| 1 | -1.872 | -0.157 | 3.849 |
| 1 | 0.486 | 0.219 | 1.960 |
| 1 | 1.428 | -2.172 | 4.816 |
| 1 | -0.476 | -2.336 | 3.331 |
| 1 | -1.523 | -0.107 | 0.913 |
| 1 | 0.750 | -2.441 | 1.258 |
| 1 | 3.023 | -0.568 | 4.384 |

$[CuCl_2]$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.367 | 0.097 | 1.657 |
| 6 | 3.066 | -0.800 | 0.812 |
| 6 | 4.185 | -0.342 | -0.095 |
| 6 | 5.551 | -0.485 | 0.609 |
| 6 | 6.033 | -1.904 | 0.897 |
| 8 | 7.236 | -1.733 | 1.627 |
| 8 | 1.447 | -0.275 | 2.506 |
| 29 | 0.075 | -1.472 | 2.107 |
| 17 | -0.349 | -0.810 | 0.037 |
| 8 | 2.701 | -2.059 | 0.847 |
| 17 | -1.304 | -3.000 | 2.724 |
| 8 | 3.961 | 1.008 | -0.396 |
| 8 | 6.444 | 0.201 | -0.247 |
| 6 | 6.307 | -2.744 | -0.342 |
| 8 | 6.916 | -3.936 | 0.132 |
| 1 | 7.370 | -4.372 | -0.597 |
| 1 | 5.290 | -2.419 | 1.526 |
| 1 | 6.978 | -2.200 | -1.015 |
| 1 | 5.378 | -2.973 | -0.882 |
| 1 | 7.297 | 0.259 | 0.201 |
| 1 | 5.484 | 0.038 | 1.573 |
| 1 | 4.170 | -0.952 | -1.012 |
| 1 | 2.794 | 1.098 | 1.746 |
| 1 | 1.951 | 0.118 | 0.459 |
| 1 | 4.822 | 1.378 | -0.646 |
| 1 | 7.703 | -2.580 | 1.582 |
| 1 | 2.946 | -2.552 | 0.048 |

$[CuCl_2]$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -1.058 | 0.170 | 0.117 |
| 8 | -1.597 | 1.479 | 0.109 |
| 6 | -0.839 | -0.269 | -1.309 |
| 6 | -0.435 | -1.734 | -1.441 |
| 8 | -1.579 | -2.521 | -1.655 |
| 8 | 0.221 | 0.494 | -1.925 |
| 6 | 0.555 | -1.721 | -2.606 |
| 8 | 1.500 | -2.756 | -2.467 |
| 6 | 1.194 | -0.334 | -2.453 |
| 8 | 2.273 | -0.456 | -1.496 |
| 29 | 3.663 | 1.012 | -1.568 |
| 17 | 4.487 | 3.056 | -1.539 |
| 6 | 1.792 | 0.299 | -3.696 |
| 8 | 2.643 | 1.384 | -3.301 |
| 17 | 4.979 | -0.024 | -0.134 |
| 1 | -1.720 | 1.767 | 1.019 |
| 1 | -0.103 | 0.134 | 0.658 |
| 1 | -1.752 | -0.542 | 0.586 |
| 1 | -1.356 | -3.446 | -1.495 |
| 1 | 1.794 | -3.064 | -3.332 |
| 1 | 0.010 | -1.783 | -3.554 |
| 1 | 2.432 | -0.418 | -4.215 |
| 1 | 2.154 | 2.217 | -3.265 |
| 1 | 1.012 | 0.654 | -4.372 |
| 1 | 0.103 | -2.068 | -0.542 |
| 1 | -1.752 | -0.091 | -1.890 |
| 1 | 2.600 | -1.377 | -1.524 |

$[CuH_2OCl]^+$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | 1.246 | -1.252 | 4.131 |
| 8 | 0.587 | -0.463 | 5.038 |
| 6 | -0.009 | 0.751 | 4.541 |
| 6 | -1.005 | 0.414 | 3.425 |
| 6 | -0.264 | -0.342 | 2.330 |
| 6 | 0.406 | -1.575 | 2.902 |
| 6 | -0.653 | 1.435 | 5.722 |
| 8 | 0.371 | 1.905 | 6.578 |
| 8 | -1.518 | 1.586 | 2.824 |
| 8 | -1.109 | -0.803 | 1.301 |
| 8 | 1.290 | -2.168 | 1.936 |
| 29 | 3.143 | -1.425 | 1.951 |
| 17 | 5.154 | -0.600 | 2.178 |
| 8 | 2.426 | -0.597 | 3.602 |
| 8 | 3.535 | -2.283 | 0.227 |
| 1 | -0.038 | 2.333 | 7.338 |
| 1 | 0.779 | 1.401 | 4.138 |
| 1 | -1.310 | 0.722 | 6.238 |
| 1 | -1.263 | 2.266 | 5.346 |
| 1 | -2.406 | 1.760 | 3.152 |
| 1 | -1.813 | -0.215 | 3.821 |
| 1 | 0.499 | 0.338 | 1.918 |
| 1 | 1.553 | -2.156 | 4.661 |
| 1 | -0.352 | -2.316 | 3.175 |
| 1 | -1.480 | -0.034 | 0.850 |
| 1 | 0.823 | -2.247 | 1.088 |
| 1 | 3.085 | -0.453 | 4.299 |
| 1 | 4.433 | -2.066 | -0.063 |
| 1 | 3.458 | -3.248 | 0.193 |

$[CuH_2OCl]^+$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.071 | 0.325 | 1.019 |
| 8 | 0.979 | -0.053 | 1.648 |
| 29 | 0.511 | -1.869 | 1.605 |
| 17 | 0.164 | -4.000 | 1.450 |
| 6 | 2.918 | -0.638 | 0.407 |
| 8 | 2.417 | -1.855 | 0.446 |
| 6 | 4.227 | -0.318 | -0.258 |
| 8 | 4.180 | 1.040 | -0.585 |
| 6 | 5.408 | -0.574 | 0.726 |
| 8 | 6.474 | 0.170 | 0.171 |
| 6 | 5.782 | -2.037 | 0.942 |
| 6 | 6.476 | -2.691 | -0.243 |
| 8 | 6.828 | -3.994 | 0.200 |
| 8 | 6.650 | -2.042 | 2.061 |
| 8 | -1.108 | -1.418 | 2.644 |
| 1 | 7.511 | -4.351 | -0.377 |
| 1 | 4.874 | -2.612 | 1.185 |
| 1 | 7.367 | -2.111 | -0.507 |
| 1 | 5.817 | -2.741 | -1.119 |
| 1 | 7.103 | 0.383 | 0.871 |
| 1 | 5.131 | -0.158 | 1.704 |
| 1 | 4.341 | -0.938 | -1.160 |
| 1 | 2.506 | 1.302 | 1.246 |
| 1 | 1.945 | 0.422 | -0.195 |
| 1 | 5.100 | 1.353 | -0.548 |
| 1 | 7.086 | -2.907 | 2.061 |
| 1 | 2.749 | -2.495 | -0.207 |
| 1 | -1.416 | -2.110 | 3.245 |
| 1 | -1.006 | -0.605 | 3.159 |

$[CuH_2OCl]^+$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | 1.189 | -0.216 | -2.416 |
| 8 | 0.181 | 0.548 | -1.867 |
| 6 | -0.858 | -0.280 | -1.298 |
| 6 | -0.373 | -1.719 | -1.441 |
| 6 | 0.636 | -1.639 | -2.588 |
| 6 | -1.141 | 0.124 | 0.128 |
| 8 | -1.742 | 1.405 | 0.122 |
| 8 | -1.469 | -2.562 | -1.688 |
| 8 | 1.642 | -2.612 | -2.429 |
| 8 | 2.287 | -0.301 | -1.463 |
| 29 | 3.622 | 1.145 | -1.599 |
| 17 | 4.818 | 0.473 | 0.110 |
| 6 | 1.750 | 0.483 | -3.641 |
| 8 | 2.502 | 1.630 | -3.199 |
| 8 | 4.874 | 2.602 | -1.998 |

| | | | |
|---|---|---|---|
| 1 | -1.898 | 1.676 | 1.033 |
| 1 | -0.202 | 0.125 | 0.698 |
| 1 | -1.812 | -0.630 | 0.563 |
| 1 | -1.206 | -3.474 | -1.520 |
| 1 | 1.971 | -2.906 | -3.287 |
| 1 | 0.115 | -1.731 | -3.548 |
| 1 | 2.457 | -0.157 | -4.171 |
| 1 | 1.902 | 2.377 | -3.053 |
| 1 | 0.955 | 0.799 | -4.317 |
| 1 | 0.166 | -2.035 | -0.537 |
| 1 | -1.760 | -0.137 | -1.905 |
| 1 | 2.634 | -1.218 | -1.498 |
| 1 | 5.472 | 2.776 | -1.257 |
| 1 | 4.535 | 3.453 | -2.306 |

$[Cu(H_2O)_2]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.025 | 0.777 | 4.548 |
| 6 | -0.991 | 0.401 | 3.419 |
| 6 | -0.228 | -0.407 | 2.376 |
| 6 | 0.407 | -1.621 | 3.021 |
| 6 | 1.206 | -1.267 | 4.266 |
| 8 | 0.553 | -0.420 | 5.113 |
| 8 | -1.471 | 1.553 | 2.756 |
| 8 | -1.046 | -0.900 | 1.344 |
| 8 | 1.326 | -2.266 | 2.117 |
| 29 | 3.143 | -1.553 | 2.147 |
| 8 | 2.435 | -0.667 | 3.748 |
| 6 | -0.698 | 1.507 | 5.685 |
| 8 | 0.304 | 2.002 | 6.552 |
| 8 | 4.929 | -0.809 | 2.321 |
| 8 | 3.707 | -2.388 | 0.470 |
| 1 | -0.125 | 2.460 | 7.283 |
| 1 | 0.778 | 1.407 | 4.143 |
| 1 | -1.373 | 0.815 | 6.207 |
| 1 | -1.293 | 2.325 | 5.261 |
| 1 | -2.371 | 1.742 | 3.039 |
| 1 | -1.819 | -0.201 | 3.817 |
| 1 | 0.554 | 0.250 | 1.963 |
| 1 | 1.477 | -2.153 | 4.844 |
| 1 | -0.365 | -2.349 | 3.288 |
| 1 | -1.399 | -0.146 | 0.853 |
| 1 | 0.888 | -2.418 | 1.263 |
| 1 | 5.504 | -1.032 | 1.574 |
| 1 | 5.435 | -0.986 | 3.128 |
| 1 | 3.340 | -2.054 | -0.361 |
| 1 | 3.704 | -3.355 | 0.421 |
| 1 | 3.030 | -0.454 | 4.484 |

$[Cu(H_2O)_2]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.318 | 0.641 | 1.206 |
| 6 | 3.051 | -0.374 | 0.529 |
| 6 | 4.328 | -0.113 | -0.237 |
| 6 | 5.566 | -0.338 | 0.637 |
| 6 | 5.790 | -1.758 | 1.154 |
| 8 | 7.045 | -1.702 | 1.822 |
| 8 | 1.324 | 0.272 | 1.956 |
| 29 | 1.222 | -1.632 | 1.955 |
| 8 | -0.327 | -1.600 | 3.184 |
| 8 | 2.676 | -1.608 | 0.726 |
| 8 | 1.169 | -3.611 | 1.917 |
| 8 | 4.301 | 1.227 | -0.674 |
| 8 | 6.651 | 0.073 | -0.177 |
| 6 | 5.835 | -2.824 | 0.070 |
| 8 | 6.310 | -4.004 | 0.708 |
| 1 | 6.628 | -4.619 | 0.039 |
| 1 | 4.996 | -2.009 | 1.870 |
| 1 | 6.517 | -2.516 | -0.732 |
| 1 | 4.833 | -2.981 | -0.345 |
| 1 | 7.460 | -0.142 | 0.309 |
| 1 | 5.489 | 0.326 | 1.511 |
| 1 | 4.355 | -0.800 | -1.095 |
| 1 | 2.620 | 1.688 | 1.158 |
| 1 | 2.151 | 0.388 | -0.129 |
| 1 | 5.207 | 1.458 | -0.921 |
| 1 | -0.273 | -2.114 | 4.001 |
| 1 | -0.573 | -0.699 | 3.437 |
| 1 | 1.804 | -3.982 | 1.289 |
| 1 | 0.320 | -4.039 | 1.744 |
| 1 | 7.364 | -2.615 | 1.869 |

$[Cu(H_2O)_2]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | 0.690 | -1.639 | -2.577 |
| 6 | 1.250 | -0.221 | -2.395 |
| 8 | 0.264 | 0.542 | -1.823 |
| 6 | -0.776 | -0.285 | -1.246 |
| 6 | -0.308 | -1.727 | -1.420 |
| 8 | 2.366 | -0.341 | -1.447 |
| 29 | 3.614 | 1.142 | -1.525 |
| 8 | 4.924 | 2.552 | -1.782 |
| 6 | 1.821 | 0.483 | -3.612 |
| 8 | 2.614 | 1.603 | -3.155 |
| 6 | -1.029 | 0.104 | 0.189 |
| 8 | -1.613 | 1.392 | 0.209 |
| 8 | -1.416 | -2.551 | -1.669 |
| 8 | 1.702 | -2.609 | -2.441 |
| 8 | 4.488 | 0.715 | 0.165 |
| 1 | -1.762 | 1.649 | 1.125 |
| 1 | -0.082 | 0.084 | 0.744 |
| 1 | -1.704 | -0.647 | 0.624 |
| 1 | -1.167 | -3.469 | -1.510 |
| 1 | 1.992 | -2.927 | -3.304 |
| 1 | 0.160 | -1.718 | -3.532 |
| 1 | 2.505 | -0.166 | -4.161 |
| 1 | 2.063 | 2.396 | -3.073 |
| 1 | 1.031 | 0.841 | -4.273 |
| 1 | 0.237 | -2.064 | -0.526 |
| 1 | -1.685 | -0.122 | -1.838 |
| 1 | 2.718 | -1.255 | -1.544 |
| 1 | 5.061 | 3.175 | -1.054 |
| 1 | 4.897 | 3.063 | -2.602 |
| 1 | 5.382 | 0.348 | 0.118 |
| 1 | 3.991 | 0.177 | 0.797 |

$[Cu(H_2O)_6]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -2.647 | -1.080 | 2.325 |
| 6 | -2.379 | -1.072 | 0.827 |
| 6 | -0.945 | -1.474 | 0.542 |
| 6 | 0.028 | -0.600 | 1.325 |
| 8 | -0.290 | -0.624 | 2.682 |
| 6 | -1.614 | -0.186 | 3.020 |
| 8 | -3.196 | -1.989 | 0.127 |
| 8 | -0.674 | -1.376 | -0.848 |
| 8 | -0.020 | 0.714 | 0.796 |
| 6 | -1.723 | -0.228 | 4.526 |
| 8 | -0.911 | 0.798 | 5.068 |
| 8 | -3.965 | -0.593 | 2.506 |
| 8 | 0.226 | 1.378 | -1.792 |
| 29 | 1.907 | 0.881 | -2.672 |
| 8 | 1.030 | 0.584 | -4.778 |
| 8 | 3.510 | 0.910 | -0.927 |
| 8 | 3.615 | 0.454 | -3.623 |
| 8 | 2.265 | 2.796 | -3.152 |
| 8 | 1.483 | -1.016 | -2.315 |
| 1 | -0.977 | 0.764 | 6.028 |
| 1 | -1.405 | -1.218 | 4.882 |
| 1 | -2.775 | -0.079 | 4.800 |
| 1 | -1.756 | 0.850 | 2.682 |
| 1 | -2.557 | -2.110 | 2.698 |
| 1 | -4.399 | -1.085 | 3.210 |
| 1 | -2.550 | -0.051 | 0.453 |
| 1 | -4.113 | -1.707 | 0.228 |
| 1 | -0.791 | -2.507 | 0.880 |
| 1 | -1.393 | -1.820 | -1.320 |
| 1 | 1.046 | -0.997 | 1.259 |
| 1 | 3.909 | 1.728 | -0.608 |
| 1 | -0.080 | 2.288 | -1.885 |
| 1 | 2.332 | 3.455 | -2.448 |
| 1 | 0.626 | 1.334 | -5.230 |
| 1 | 4.313 | 0.162 | -3.019 |
| 1 | 0.715 | -1.206 | -1.714 |
| 1 | 0.390 | -0.135 | -4.838 |
| 1 | 2.201 | -1.614 | -2.073 |
| 1 | 3.564 | -0.168 | -4.360 |
| 1 | 3.370 | 0.370 | -0.140 |
| 1 | 0.100 | 1.106 | -0.846 |
| 1 | 3.067 | 2.881 | -3.686 |
| 1 | 0.622 | 1.255 | 1.277 |

$[Cu(H_2O)_6]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | -0.483 | -0.835 | 2.285 |
| 6 | -0.342 | -1.457 | 3.563 |
| 8 | 0.452 | -2.482 | 3.695 |
| 8 | 0.048 | -1.287 | 1.187 |
| 6 | -1.093 | -0.951 | 4.782 |
| 8 | -2.147 | -1.875 | 4.915 |
| 6 | -0.183 | -0.870 | 6.021 |
| 8 | 0.392 | -2.172 | 6.196 |
| 6 | -0.947 | -0.395 | 7.254 |
| 6 | -0.085 | -0.276 | 8.505 |
| 8 | -0.908 | 0.042 | 9.614 |
| 8 | -2.014 | -1.298 | 7.499 |
| 8 | 2.000 | -2.755 | 0.778 |
| 29 | 1.213 | -4.425 | 0.173 |
| 8 | 2.873 | -5.950 | 0.722 |
| 8 | -0.732 | -3.360 | -0.329 |
| 8 | 0.445 | -4.822 | 2.009 |
| 8 | 2.183 | -4.142 | -1.581 |
| 8 | 0.482 | -6.094 | -0.632 |
| 1 | -1.348 | 0.602 | 7.011 |
| 1 | -1.325 | -0.131 | 2.223 |
| 1 | -1.103 | 0.987 | 9.601 |
| 1 | 0.708 | 0.467 | 8.359 |
| 1 | 0.373 | -1.242 | 8.741 |
| 1 | 1.215 | -2.114 | 6.699 |
| 1 | 0.604 | -0.135 | 5.811 |
| 1 | -1.462 | 0.063 | 4.573 |
| 1 | 0.597 | -2.627 | 4.685 |
| 1 | -2.403 | -1.062 | 8.354 |
| 1 | -2.451 | -1.833 | 5.842 |
| 1 | 2.390 | -3.213 | -1.749 |
| 1 | 1.734 | -4.483 | -2.366 |
| 1 | 0.943 | -6.871 | -0.285 |
| 1 | -0.467 | -6.271 | -0.612 |
| 1 | 3.725 | -5.877 | 0.275 |
| 1 | -0.680 | -2.506 | 0.159 |
| 1 | 3.071 | -6.088 | 1.656 |
| 1 | -0.920 | -3.141 | -1.248 |

| | | | |
|---|---|---|---|
| 1 | 0.427 | -4.045 | 2.597 |
| 1 | 2.681 | -2.810 | 1.458 |
| 1 | 1.260 | -2.086 | 1.073 |
| 1 | -0.453 | -5.178 | 2.011 |
| 1 | 0.287 | -0.174 | 2.996 |

$[Cu(H_2O)_6]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.201 | 0.053 | -5.049 |
| 8 | -0.094 | 0.840 | -3.848 |
| 6 | 1.079 | 1.608 | -3.847 |
| 6 | 1.279 | 1.932 | -5.343 |
| 6 | 0.769 | 0.686 | -6.063 |
| 6 | 0.766 | 2.768 | -2.911 |
| 8 | 1.926 | 3.533 | -2.621 |
| 8 | 2.168 | 0.878 | -3.325 |
| 8 | 2.631 | 2.235 | -5.667 |
| 8 | 0.163 | 1.079 | -7.276 |
| 6 | 0.092 | -1.399 | -4.734 |
| 8 | 1.460 | -1.501 | -4.337 |
| 8 | 4.229 | 3.586 | -3.931 |
| 29 | 5.631 | 2.341 | -3.339 |
| 8 | 7.177 | 1.152 | -2.882 |
| 8 | 6.565 | 3.490 | -1.540 |
| 8 | 5.010 | 0.793 | -4.938 |
| 8 | 4.377 | 1.534 | -2.030 |
| 8 | 6.932 | 3.347 | -4.496 |
| 1 | 1.622 | -2.358 | -3.929 |
| 1 | -0.570 | -1.739 | -3.930 |
| 1 | -0.089 | -2.009 | -5.628 |
| 1 | -1.230 | 0.140 | -5.410 |
| 1 | 1.614 | 0.016 | -6.258 |
| 1 | -0.006 | 3.391 | -3.377 |
| 1 | 3.487 | 3.687 | -3.288 |
| 1 | 3.751 | 3.231 | -4.712 |
| 1 | 0.633 | 2.777 | -5.608 |
| 1 | 2.661 | 2.509 | -6.594 |
| 1 | 0.132 | 0.325 | -7.875 |
| 1 | 5.575 | 0.658 | -5.708 |
| 1 | 4.129 | 1.012 | -5.288 |
| 1 | 2.063 | -0.066 | -3.600 |
| 1 | 7.020 | 4.318 | -1.738 |
| 1 | 5.987 | 3.677 | -0.791 |
| 1 | 4.698 | 0.760 | -1.551 |
| 1 | 7.549 | 1.367 | -2.014 |
| 1 | 7.079 | 0.192 | -2.937 |
| 1 | 3.508 | 1.287 | -2.443 |
| 1 | 7.657 | 2.818 | -4.855 |
| 1 | 6.560 | 3.856 | -5.228 |
| 1 | 0.365 | 2.329 | -1.991 |
| 1 | 1.696 | 4.220 | -1.986 |

$[Al(H_2O)_6]^{3+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.504 | -1.845 | 0.962 |
| 6 | 0.344 | -1.052 | 1.961 |
| 8 | -0.417 | -0.701 | 3.071 |
| 6 | -1.587 | 0.078 | 2.794 |
| 6 | -2.525 | -0.723 | 1.896 |
| 6 | -1.801 | -1.129 | 0.618 |
| 8 | 0.900 | 0.091 | 1.321 |
| 6 | -2.220 | 0.425 | 4.121 |
| 8 | -1.382 | 1.352 | 4.789 |
| 8 | -3.648 | 0.074 | 1.593 |
| 8 | -2.684 | -1.965 | -0.099 |
| 8 | 0.201 | -2.141 | -0.242 |
| 8 | 0.769 | 1.323 | -0.893 |
| 13 | 1.659 | 0.811 | -2.462 |
| 8 | 2.605 | 0.381 | -4.066 |
| 8 | 2.381 | 2.575 | -2.568 |
| 8 | 0.945 | -0.917 | -2.359 |
| 8 | 0.196 | 1.352 | -3.565 |
| 8 | 3.213 | 0.273 | -1.486 |
| 1 | -1.791 | 1.581 | 5.630 |
| 1 | -2.345 | -0.494 | 4.710 |
| 1 | -3.210 | 0.854 | 3.926 |
| 1 | -1.297 | 1.009 | 2.287 |
| 1 | -2.832 | -1.639 | 2.426 |
| 1 | -4.178 | -0.411 | 0.947 |
| 1 | -1.598 | -0.215 | 0.042 |
| 1 | -2.367 | -2.062 | -1.005 |
| 1 | -0.763 | -2.789 | 1.454 |
| 1 | 0.749 | -2.927 | -0.124 |
| 1 | 1.161 | -1.669 | 2.345 |
| 1 | 3.866 | 0.888 | -1.123 |
| 1 | -0.030 | 1.867 | -0.923 |
| 1 | 2.246 | 3.266 | -1.905 |
| 1 | 0.049 | 2.234 | -3.933 |
| 1 | 3.495 | 0.001 | -4.100 |
| 1 | 0.605 | -1.360 | -1.514 |
| 1 | -0.592 | 0.807 | -3.702 |
| 1 | 1.132 | -1.592 | -3.025 |
| 1 | 2.239 | 0.435 | -4.960 |
| 1 | 3.372 | -0.610 | -1.124 |
| 1 | 0.805 | 0.825 | -0.010 |
| 1 | 2.956 | 2.906 | -3.272 |
| 1 | 1.553 | 0.497 | 1.907 |

$[Al(H_2O)_6]^{3+}$-TS2

| | | | |
|---|---|---|---|
| 6 | -0.247 | -0.473 | 2.294 |
| 8 | 0.253 | -0.776 | 1.124 |
| 6 | -0.175 | -1.221 | 3.492 |
| 6 | -0.959 | -0.774 | 4.720 |
| 6 | -0.109 | -0.879 | 6.000 |
| 6 | -0.911 | -0.490 | 7.238 |
| 8 | -2.032 | -1.356 | 7.338 |
| 8 | 0.501 | -2.343 | 3.558 |
| 8 | -2.077 | -1.624 | 4.708 |
| 8 | 0.382 | -2.226 | 6.061 |
| 6 | -0.110 | -0.546 | 8.534 |
| 8 | -0.972 | -0.296 | 9.631 |
| 8 | 1.661 | -2.773 | 0.678 |
| 13 | 1.121 | -4.423 | 0.261 |
| 8 | -0.565 | -3.825 | -0.491 |
| 8 | 0.301 | -4.639 | 1.968 |
| 8 | 1.918 | -4.333 | -1.482 |
| 8 | 0.483 | -6.180 | -0.228 |
| 8 | 2.680 | -5.389 | 0.903 |
| 1 | -1.250 | 0.546 | 7.080 |
| 1 | -0.950 | 0.360 | 2.301 |
| 1 | -1.106 | 0.655 | 9.719 |
| 1 | 0.726 | 0.164 | 8.502 |
| 1 | 0.286 | -1.554 | 8.689 |
| 1 | 1.190 | -2.269 | 6.589 |
| 1 | 0.729 | -0.177 | 5.908 |
| 1 | -1.243 | 0.281 | 4.598 |
| 1 | 0.603 | -2.558 | 4.545 |
| 1 | -2.462 | -1.177 | 8.187 |
| 1 | -2.417 | -1.668 | 5.624 |
| 1 | 2.380 | -3.542 | -1.793 |
| 1 | 1.884 | -4.997 | -2.184 |
| 1 | 0.936 | -7.009 | -0.023 |
| 1 | -0.372 | -6.360 | -0.640 |
| 1 | 3.516 | -5.408 | 0.415 |
| 1 | -1.321 | -3.597 | 0.068 |
| 1 | 2.871 | -5.472 | 1.848 |
| 1 | -0.593 | -3.267 | -1.280 |
| 1 | 0.292 | -3.875 | 2.579 |
| 1 | 2.558 | -2.645 | 1.005 |
| 1 | 0.836 | -1.634 | 1.033 |
| 1 | -0.277 | -5.345 | 2.287 |
| 1 | 0.601 | -0.055 | 3.160 |

$[Al(H_2O)_6]^{3+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.997 | 0.746 | 1.306 |
| 8 | -2.109 | 0.774 | 2.148 |
| 6 | -3.351 | 0.747 | 1.407 |
| 6 | -2.935 | 0.645 | -0.061 |
| 6 | -1.543 | 1.257 | -0.034 |
| 6 | -4.227 | -0.384 | 1.884 |
| 8 | -4.651 | -0.099 | 3.203 |
| 8 | -3.745 | 1.370 | -0.954 |
| 8 | -0.766 | 0.889 | -1.157 |
| 6 | 0.053 | 1.577 | 2.043 |
| 8 | 1.361 | 1.347 | 1.530 |
| 8 | -0.556 | -0.597 | 1.106 |
| 8 | 1.086 | -1.736 | -0.546 |
| 13 | 2.507 | -0.841 | -1.387 |
| 8 | 3.931 | 0.089 | -2.252 |
| 8 | 1.794 | 0.813 | -0.925 |
| 8 | 1.546 | -0.881 | -3.045 |
| 8 | 3.302 | -2.499 | -1.915 |
| 8 | 3.576 | -0.953 | 0.202 |
| 1 | -5.192 | -0.832 | 3.518 |
| 1 | -3.662 | -1.325 | 1.838 |
| 1 | -5.086 | -0.462 | 1.201 |
| 1 | -4.411 | 0.787 | -1.334 |
| 1 | -1.222 | 1.195 | -1.954 |
| 1 | 0.671 | -1.278 | -3.162 |
| 1 | -1.633 | 2.349 | 0.027 |
| 1 | -0.219 | 2.634 | 1.964 |
| 1 | 1.992 | 1.887 | 2.022 |
| 1 | 0.020 | 1.281 | 3.096 |
| 1 | -0.428 | -1.009 | 1.974 |
| 1 | 3.124 | -2.963 | -2.745 |
| 1 | 3.926 | -3.009 | -1.380 |
| 1 | 4.672 | -0.298 | -2.738 |
| 1 | 4.414 | -0.487 | 0.332 |
| 1 | 3.252 | -1.272 | 1.056 |
| 1 | 3.970 | 1.054 | -2.300 |
| 1 | -2.850 | -0.405 | -0.372 |
| 1 | -3.858 | 1.705 | 1.577 |
| 1 | 1.801 | -0.416 | -3.854 |
| 1 | 0.418 | -1.277 | 0.052 |
| 1 | 1.766 | 1.081 | 0.048 |
| 1 | 0.992 | -2.696 | -0.484 |
| 1 | 0.848 | 0.968 | -1.211 |

$[Al(H_2O)_4]^{3+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -1.095 | 0.487 | 3.448 |
| 6 | -0.490 | -0.240 | 2.267 |
| 6 | 0.848 | 0.334 | 1.813 |
| 8 | 1.671 | 0.736 | 2.807 |
| 6 | 1.116 | 1.504 | 3.901 |
| 6 | -0.037 | 0.714 | 4.525 |
| 8 | -1.363 | -0.144 | 1.107 |
| 13 | -1.009 | 1.140 | -0.252 |
| 8 | -0.046 | -0.208 | -1.215 |
| 8 | 0.461 | 1.472 | 0.933 |
| 6 | 2.252 | 1.766 | 4.858 |
| 8 | 3.153 | 2.662 | 4.238 |

| | | | |
|---|---|---|---|
| 8 | -0.674 | 1.449 | 5.546 |
| 8 | -2.171 | -0.299 | 3.889 |
| 8 | -2.530 | 0.671 | -1.274 |
| 8 | -2.084 | 2.478 | 0.586 |
| 8 | -0.438 | 2.421 | -1.524 |
| 1 | 3.876 | 2.841 | 4.849 |
| 1 | 0.744 | 2.462 | 3.515 |
| 1 | 2.740 | 0.815 | 5.110 |
| 1 | 1.830 | 2.198 | 5.774 |
| 1 | -0.399 | 1.120 | 6.408 |
| 1 | 0.329 | -0.252 | 4.896 |
| 1 | -1.443 | 1.482 | 3.133 |
| 1 | 1.408 | -0.365 | 1.189 |
| 1 | -0.365 | -1.301 | 2.500 |
| 1 | -2.588 | 0.159 | 4.630 |
| 1 | -2.182 | -0.651 | 1.220 |
| 1 | -2.836 | 2.344 | 1.180 |
| 1 | -2.029 | 3.418 | 0.360 |
| 1 | -0.953 | 2.605 | -2.325 |
| 1 | 0.350 | 2.986 | -1.534 |
| 1 | 0.495 | -0.030 | -1.998 |
| 1 | -0.142 | -1.167 | -1.110 |
| 1 | -3.390 | 1.116 | -1.251 |
| 1 | -2.544 | -0.014 | -1.959 |
| 1 | 1.260 | 1.973 | 0.704 |

$[Al(H_2O)_4]^{3+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 0.499 | -1.395 | 3.388 |
| 6 | 0.480 | -0.955 | 1.911 |
| 6 | 0.876 | 0.487 | 1.739 |
| 6 | 2.209 | 0.936 | 1.522 |
| 8 | 0.309 | 0.432 | 4.955 |
| 6 | -0.447 | -0.600 | 4.302 |
| 8 | 1.386 | -1.734 | 1.173 |
| 8 | -0.012 | 1.425 | 1.956 |
| 13 | 0.842 | 3.062 | 2.178 |
| 8 | 1.865 | 4.682 | 2.280 |
| 8 | 2.397 | 2.223 | 1.568 |
| 6 | -1.064 | -1.461 | 5.395 |
| 8 | -1.694 | -0.542 | 6.278 |
| 8 | 0.147 | -2.768 | 3.317 |
| 8 | 0.252 | 3.670 | 0.409 |
| 8 | -0.703 | 4.052 | 2.767 |
| 8 | 1.090 | 2.684 | 4.035 |
| 1 | -1.837 | -0.964 | 7.132 |
| 1 | -1.253 | -0.129 | 3.723 |
| 1 | -0.284 | -2.024 | 5.922 |
| 1 | -1.784 | -2.161 | 4.962 |
| 1 | 0.665 | -3.271 | 3.955 |
| 1 | 1.520 | -1.279 | 3.775 |
| 1 | -0.548 | -1.067 | 1.536 |
| 1 | 3.041 | 0.246 | 1.398 |
| 1 | 1.414 | 0.516 | 0.499 |
| 1 | 1.245 | -2.651 | 1.450 |
| 1 | 0.781 | 1.778 | 4.378 |
| 1 | 1.870 | 2.969 | 4.526 |
| 1 | 1.583 | 5.486 | 2.736 |
| 1 | 2.829 | 4.677 | 2.195 |
| 1 | 0.776 | 4.296 | -0.108 |
| 1 | -0.183 | 3.059 | -0.202 |
| 1 | -1.067 | 3.936 | 3.656 |
| 1 | -1.403 | 4.333 | 2.163 |
| 1 | -0.191 | 0.624 | 5.771 |

$[Al(H_2O)_4]^{3+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -1.859 | -1.724 | 1.337 |
| 6 | -2.610 | -0.897 | 2.246 |
| 6 | -2.378 | 0.566 | 1.926 |
| 6 | -2.769 | 0.987 | 0.501 |
| 6 | -1.485 | 1.630 | -0.041 |
| 6 | -0.395 | 0.966 | 0.810 |
| 8 | -0.958 | 0.842 | 2.054 |
| 6 | 0.960 | 1.646 | 0.944 |
| 8 | 1.784 | 1.216 | -0.165 |
| 13 | 1.488 | -0.622 | -0.707 |
| 8 | -3.865 | 1.862 | 0.563 |
| 8 | -1.293 | 1.438 | -1.430 |
| 8 | -0.090 | -0.357 | 0.266 |
| 8 | 0.571 | -0.121 | -2.275 |
| 8 | 1.143 | -2.422 | -1.183 |
| 8 | 2.374 | -1.252 | 0.871 |
| 8 | 3.173 | -0.650 | -1.587 |
| 1 | -2.437 | -2.289 | 0.811 |
| 1 | -3.675 | -1.130 | 2.174 |
| 1 | -2.262 | -1.117 | 3.258 |
| 1 | -4.308 | 1.879 | -0.293 |
| 1 | -1.499 | 2.244 | -1.918 |
| 1 | -0.207 | 0.490 | -2.094 |
| 1 | -1.497 | 2.698 | 0.200 |
| 1 | 0.885 | 2.732 | 0.944 |
| 1 | 1.923 | 1.928 | -0.806 |
| 1 | 1.446 | 1.306 | 1.860 |
| 1 | -0.786 | -1.044 | 0.636 |
| 1 | 0.544 | -2.674 | -1.900 |
| 1 | 1.410 | -3.207 | -0.685 |
| 1 | 3.462 | -1.372 | -2.165 |
| 1 | 3.324 | -1.431 | 0.930 |
| 1 | 1.941 | -1.567 | 1.676 |
| 1 | 3.866 | 0.024 | -1.553 |
| 1 | -3.005 | 0.112 | -0.119 |
| 1 | -2.898 | 1.189 | 2.658 |
| 1 | 0.990 | 0.101 | -3.117 |

$[Al(H_2O)_3Cl]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.046 | 0.755 | 4.536 |
| 6 | -1.101 | 0.463 | 3.477 |
| 6 | -0.494 | -0.277 | 2.302 |
| 6 | 0.845 | 0.285 | 1.833 |
| 8 | 1.663 | 0.730 | 2.820 |
| 6 | 1.096 | 1.533 | 3.878 |
| 8 | -2.147 | -0.349 | 3.951 |
| 8 | -1.358 | -0.205 | 1.149 |
| 13 | -1.113 | 1.164 | -0.210 |
| 8 | -1.887 | 2.588 | 0.849 |
| 8 | 0.473 | 1.365 | 0.896 |
| 6 | 2.228 | 1.850 | 4.825 |
| 8 | 3.120 | 2.731 | 4.172 |
| 8 | -0.691 | 1.524 | 5.529 |
| 8 | -0.184 | -0.062 | -1.393 |
| 17 | -3.024 | 0.728 | -1.151 |
| 8 | -0.408 | 2.535 | -1.371 |
| 1 | 3.843 | 2.937 | 4.775 |
| 1 | 0.714 | 2.472 | 3.456 |
| 1 | 2.727 | 0.915 | 5.115 |
| 1 | 1.800 | 2.313 | 5.723 |
| 1 | -0.395 | 1.247 | 6.402 |
| 1 | 0.337 | -0.187 | 4.949 |
| 1 | -1.499 | 1.429 | 3.136 |
| 1 | 1.412 | -0.452 | 1.262 |
| 1 | -0.361 | -1.331 | 2.563 |
| 1 | -2.597 | 0.131 | 4.658 |
| 1 | -2.225 | -0.607 | 1.316 |
| 1 | -0.096 | 2.295 | -2.255 |
| 1 | -0.807 | 3.416 | -1.418 |
| 1 | 0.746 | -0.325 | -1.411 |
| 1 | -0.700 | -0.700 | -1.907 |
| 1 | 1.263 | 1.832 | 0.579 |
| 1 | -1.416 | 3.304 | 1.299 |
| 1 | -2.816 | 2.836 | 0.737 |

$[Al(H_2O)_3Cl]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.138 | 0.983 | 1.349 |
| 8 | 2.415 | 2.251 | 1.500 |
| 13 | 1.084 | 3.202 | 2.386 |
| 17 | -0.494 | 4.282 | 3.459 |
| 6 | 0.952 | 0.510 | 1.960 |
| 8 | 0.245 | 1.440 | 2.567 |
| 6 | 0.508 | -0.932 | 1.991 |
| 8 | 1.476 | -1.658 | 1.294 |
| 6 | 0.338 | -1.505 | 3.429 |
| 8 | 0.198 | -2.895 | 3.233 |
| 6 | -0.928 | -1.017 | 4.133 |
| 6 | -1.249 | -1.706 | 5.443 |
| 8 | -2.310 | -0.937 | 5.989 |
| 8 | -0.738 | 0.388 | 4.491 |
| 8 | 2.073 | 4.800 | 1.895 |
| 8 | 2.081 | 2.968 | 4.056 |
| 8 | 0.128 | 3.321 | 0.654 |
| 1 | -2.358 | -1.077 | 6.941 |
| 1 | -1.793 | -1.075 | 3.463 |
| 1 | -0.372 | -1.699 | 6.101 |
| 1 | -1.553 | -2.739 | 5.248 |
| 1 | 0.794 | -3.373 | 3.822 |
| 1 | 1.222 | -1.271 | 4.034 |
| 1 | -0.473 | -0.998 | 1.495 |
| 1 | 2.855 | 0.298 | 0.903 |
| 1 | 1.086 | 0.769 | 0.587 |
| 1 | 1.260 | -2.595 | 1.414 |
| 1 | 3.023 | 2.750 | 4.048 |
| 1 | 1.892 | 3.518 | 4.828 |
| 1 | -1.503 | 0.679 | 5.030 |
| 1 | -0.444 | 0.986 | 3.651 |
| 1 | -0.804 | 3.584 | 0.666 |
| 1 | 0.555 | 3.796 | -0.073 |
| 1 | 3.012 | 4.743 | 1.670 |
| 1 | 1.904 | 5.648 | 2.326 |

$[Al(H_2O)_3Cl]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.195 | 0.801 | 0.639 |
| 8 | -0.732 | 0.606 | 1.890 |
| 6 | -2.163 | 0.399 | 1.782 |
| 6 | -2.570 | 0.933 | 0.398 |
| 6 | -1.277 | 1.578 | -0.119 |
| 6 | -2.464 | -1.066 | 2.009 |
| 8 | -1.863 | -1.814 | 0.943 |
| 8 | -3.640 | 1.834 | 0.547 |
| 8 | -1.126 | 1.507 | -1.524 |
| 6 | 1.192 | 1.415 | 0.791 |
| 8 | 1.998 | 1.012 | -0.338 |
| 13 | 1.612 | -0.818 | -1.008 |
| 8 | 2.585 | -1.320 | 0.624 |
| 8 | 0.033 | -0.475 | -0.014 |
| 8 | 3.254 | -0.759 | -2.030 |
| 8 | 0.720 | -0.050 | -2.511 |
| 17 | 1.188 | -2.910 | -1.463 |
| 1 | -2.055 | -1.381 | 2.972 |
| 1 | -3.548 | -1.223 | 2.002 |
| 1 | -4.096 | 1.923 | -0.297 |

| | | | |
|---|---|---|---|
| 1 | -1.280 | 2.372 | -1.922 |
| 1 | -0.028 | 0.571 | -2.289 |
| 1 | -1.247 | 2.619 | 0.220 |
| 1 | 1.161 | 2.502 | 0.848 |
| 1 | 2.133 | 1.748 | -0.951 |
| 1 | 1.660 | 1.007 | 1.687 |
| 1 | -0.651 | -1.162 | 0.326 |
| 1 | 3.464 | -0.979 | 0.842 |
| 1 | 2.563 | -2.257 | 0.867 |
| 1 | -2.846 | 0.112 | -0.275 |
| 1 | -2.640 | 0.994 | 2.565 |
| 1 | 1.163 | 0.213 | -3.327 |
| 1 | -1.808 | -2.749 | 1.172 |
| 1 | 3.618 | -1.592 | -2.361 |
| 1 | 3.978 | -0.125 | -1.932 |

$[Al(H_2O)_3OH]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.082 | 0.741 | 4.584 |
| 6 | -1.107 | 0.447 | 3.484 |
| 6 | -0.378 | -0.229 | 2.331 |
| 6 | 0.327 | -1.481 | 2.809 |
| 6 | 1.150 | -1.258 | 4.073 |
| 8 | 0.524 | -0.495 | 5.013 |
| 8 | -1.658 | 1.638 | 2.961 |
| 8 | -1.228 | -0.648 | 1.290 |
| 8 | 1.250 | -1.942 | 1.790 |
| 13 | 3.152 | -1.441 | 1.971 |
| 8 | 4.831 | -1.197 | 2.370 |
| 8 | 2.378 | -0.640 | 3.579 |
| 6 | -0.689 | 1.373 | 5.813 |
| 8 | 0.362 | 1.793 | 6.662 |
| 8 | 2.761 | 0.247 | 1.062 |
| 8 | 3.305 | -3.162 | 2.866 |
| 8 | 3.449 | -2.187 | 0.206 |
| 1 | -0.022 | 2.192 | 7.450 |
| 1 | 0.697 | 1.407 | 4.190 |
| 1 | -1.339 | 0.640 | 6.312 |
| 1 | -1.302 | 2.224 | 5.492 |
| 1 | -2.541 | 1.775 | 3.321 |
| 1 | -1.890 | -0.218 | 3.871 |
| 1 | 0.365 | 0.485 | 1.948 |
| 1 | 1.421 | -2.199 | 4.556 |
| 1 | -0.400 | -2.277 | 2.987 |
| 1 | -1.613 | 0.137 | 0.881 |
| 1 | 0.776 | -1.966 | 0.942 |
| 1 | 5.299 | -0.381 | 2.183 |
| 1 | 4.221 | -3.389 | 3.083 |
| 1 | 2.824 | -3.967 | 2.634 |
| 1 | 3.014 | -0.511 | 4.301 |
| 1 | 2.974 | 1.090 | 1.487 |
| 1 | 2.934 | 0.338 | 0.114 |
| 1 | 4.394 | -2.263 | 0.003 |
| 1 | 2.999 | -2.938 | -0.206 |

$[Al(H_2O)_3OH]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.230 | 0.949 | 1.459 |
| 8 | 2.455 | 2.232 | 1.411 |
| 13 | 0.995 | 3.332 | 1.799 |
| 8 | 1.200 | 3.255 | 3.772 |
| 6 | 0.898 | 0.551 | 1.740 |
| 8 | 0.067 | 1.563 | 1.864 |
| 6 | 0.424 | -0.872 | 1.920 |
| 8 | 1.567 | -1.673 | 1.886 |
| 6 | -0.374 | -1.114 | 3.236 |
| 8 | -0.445 | -2.519 | 3.343 |
| 6 | -1.810 | -0.590 | 3.174 |
| 6 | -2.697 | -0.996 | 4.332 |
| 8 | -3.886 | -0.246 | 4.141 |
| 8 | -1.766 | 0.868 | 3.222 |
| 8 | 1.751 | 4.916 | 1.727 |
| 8 | 0.298 | 3.492 | -0.041 |
| 8 | -0.791 | 4.013 | 2.281 |
| 1 | -4.378 | -0.201 | 4.968 |
| 1 | -2.282 | -0.879 | 2.228 |
| 1 | -2.216 | -0.746 | 5.285 |
| 1 | -2.882 | -2.073 | 4.288 |
| 1 | -0.181 | -2.796 | 4.228 |
| 1 | 0.157 | -0.672 | 4.088 |
| 1 | -0.254 | -1.115 | 1.086 |
| 1 | 3.043 | 0.226 | 1.453 |
| 1 | 1.519 | 0.507 | 0.464 |
| 1 | 1.281 | -2.570 | 2.115 |
| 1 | 1.207 | 2.475 | 4.342 |
| 1 | 2.685 | 4.949 | 1.509 |
| 1 | 0.758 | 4.133 | -0.600 |
| 1 | -0.088 | 2.806 | -0.600 |
| 1 | -1.256 | 4.533 | 1.611 |
| 1 | -0.868 | 4.475 | 3.126 |
| 1 | -2.678 | 1.216 | 3.240 |
| 1 | -1.045 | 1.293 | 2.515 |
| 1 | 1.867 | 3.876 | 4.096 |

$[Al(H_2O)_3OH]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.732 | 0.616 | 1.870 |
| 6 | -2.157 | 0.365 | 1.764 |
| 6 | -2.580 | 0.875 | 0.377 |
| 6 | -1.311 | 1.558 | -0.144 |
| 6 | -0.200 | 0.819 | 0.616 |
| 6 | -2.417 | -1.107 | 1.998 |
| 1 | -1.992 | -1.408 | 2.960 |
| 8 | -3.680 | 1.741 | 0.518 |
| 8 | -1.184 | 1.496 | -1.551 |
| 6 | 1.155 | 1.500 | 0.756 |
| 8 | 1.916 | 1.082 | -0.386 |
| 13 | 1.664 | -0.734 | -1.083 |
| 8 | 3.234 | -0.656 | -1.853 |
| 8 | 0.077 | -0.453 | -0.022 |
| 8 | 0.612 | -0.114 | -2.574 |
| 8 | 0.971 | -2.496 | -1.517 |
| 8 | 2.465 | -1.609 | 0.476 |
| 8 | -1.805 | -1.842 | 0.930 |
| 1 | -3.496 | -1.291 | 2.001 |
| 1 | -4.123 | 1.826 | -0.334 |
| 1 | -1.207 | 2.384 | -1.927 |
| 1 | -0.118 | 0.511 | -2.311 |
| 1 | -1.313 | 2.598 | 0.196 |
| 1 | 1.061 | 2.586 | 0.759 |
| 1 | 2.809 | 1.454 | -0.401 |
| 1 | 1.636 | 1.158 | 1.676 |
| 1 | -0.599 | -1.149 | 0.299 |
| 1 | 0.557 | -2.646 | -2.378 |
| 1 | 1.444 | -3.296 | -1.251 |
| 1 | 3.487 | -1.276 | -2.540 |
| 1 | 3.432 | -1.632 | 0.489 |
| 1 | 2.122 | -1.723 | 1.371 |
| 1 | -2.830 | 0.040 | -0.290 |
| 1 | -2.651 | 0.950 | 2.543 |
| 1 | 1.114 | 0.269 | -3.305 |
| 1 | -1.728 | -2.775 | 1.161 |

$[Al_2(H_2O)_7OH]^{5+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.193 | 0.925 | 1.487 |
| 8 | 2.318 | 2.216 | 1.567 |
| 13 | 0.592 | 3.111 | 2.139 |
| 8 | 1.025 | 2.740 | 3.987 |
| 6 | 0.856 | 0.476 | 1.650 |
| 8 | -0.042 | 1.403 | 1.940 |
| 6 | 0.513 | -0.973 | 1.908 |
| 8 | 1.442 | -1.740 | 1.190 |
| 6 | 0.573 | -1.333 | 3.405 |
| 8 | 0.289 | -2.722 | 3.410 |
| 6 | -0.401 | -0.538 | 4.293 |
| 6 | -1.003 | -1.387 | 5.404 |
| 8 | -1.634 | -0.457 | 6.276 |
| 8 | 0.324 | 0.529 | 4.934 |
| 8 | 1.854 | 4.474 | 2.036 |
| 8 | 0.058 | 3.523 | 0.328 |
| 8 | -0.953 | 4.049 | 2.730 |
| 1 | -1.762 | -0.862 | 7.140 |
| 1 | -1.211 | -0.096 | 3.700 |
| 1 | -0.217 | -1.936 | 5.935 |
| 1 | -1.719 | -2.099 | 4.986 |
| 1 | 0.851 | -3.169 | 4.052 |
| 1 | 1.591 | -1.149 | 3.772 |
| 1 | -0.514 | -1.139 | 1.553 |
| 1 | 3.038 | 0.277 | 1.264 |
| 1 | 1.216 | 0.485 | 0.446 |
| 1 | 1.347 | -2.652 | 1.501 |
| 1 | 0.696 | 1.820 | 4.356 |
| 1 | 0.884 | 3.411 | 4.672 |
| 1 | 1.682 | 5.372 | 2.341 |
| 13 | 3.511 | 3.703 | 1.695 |
| 1 | 0.226 | 4.356 | -0.132 |
| 1 | -0.588 | 3.004 | -0.172 |
| 1 | -1.420 | 3.878 | 3.561 |
| 1 | -1.563 | 4.489 | 2.122 |
| 1 | -0.172 | 0.695 | 5.760 |
| 8 | 4.538 | 5.295 | 1.850 |
| 8 | 5.104 | 2.701 | 1.384 |
| 8 | 3.801 | 3.224 | 3.539 |
| 8 | 3.490 | 3.969 | -0.206 |
| 1 | 5.546 | 2.158 | 2.053 |
| 1 | 3.112 | 3.370 | -0.865 |
| 1 | 3.008 | 2.913 | 4.017 |
| 1 | 5.498 | 5.314 | 1.723 |
| 1 | 4.324 | 3.774 | 4.141 |
| 1 | 4.252 | 6.156 | 2.186 |
| 1 | 3.602 | 4.842 | -0.607 |
| 1 | 5.518 | 2.562 | 0.521 |

$[Cr(H_2O)_4]^{3+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.047 | 0.741 | 4.523 |
| 6 | -1.070 | 0.489 | 3.419 |
| 6 | -0.431 | -0.283 | 2.287 |
| 6 | 0.900 | 0.304 | 1.838 |
| 8 | 1.711 | 0.701 | 2.845 |
| 6 | 1.141 | 1.492 | 3.915 |
| 8 | -2.170 | -0.277 | 3.838 |
| 8 | -1.291 | -0.280 | 1.115 |
| 24 | -1.016 | 1.136 | -0.245 |
| 8 | -0.550 | 2.558 | -1.536 |
| 8 | 0.506 | 1.458 | 0.985 |
| 6 | 2.258 | 1.749 | 4.896 |
| 8 | 3.188 | 2.622 | 4.287 |
| 8 | -0.701 | 1.528 | 5.494 |
| 8 | 0.004 | -0.216 | -1.262 |
| 8 | -2.566 | 0.761 | -1.415 |
| 8 | -2.068 | 2.499 | 0.747 |

| | | | |
|---|---|---|---|
| 1 | 3.898 | 2.800 | 4.913 |
| 1 | 0.799 | 2.451 | 3.505 |
| 1 | 2.724 | 0.794 | 5.173 |
| 1 | 1.820 | 2.200 | 5.795 |
| 1 | -0.481 | 1.211 | 6.376 |
| 1 | 0.289 | -0.216 | 4.944 |
| 1 | -1.399 | 1.474 | 3.055 |
| 1 | 1.467 | -0.381 | 1.206 |
| 1 | -0.284 | -1.328 | 2.572 |
| 1 | -2.651 | 0.226 | 4.507 |
| 1 | -2.165 | -0.650 | 1.334 |
| 1 | -2.940 | 2.361 | 1.146 |
| 1 | -2.005 | 3.426 | 0.470 |
| 1 | -1.076 | 2.658 | -2.344 |
| 1 | 0.318 | 2.964 | -1.679 |
| 1 | 0.474 | -0.039 | -2.091 |
| 1 | -0.108 | -1.173 | -1.156 |
| 1 | -3.479 | 1.017 | -1.214 |
| 1 | -2.589 | -0.019 | -1.991 |
| 1 | 1.309 | 1.925 | 0.695 |

$[Cr(H_2O)_4]^{3+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 0.488 | -1.421 | 3.396 |
| 6 | 0.477 | -0.979 | 1.920 |
| 6 | 0.887 | 0.461 | 1.747 |
| 6 | 2.217 | 0.903 | 1.528 |
| 8 | 0.306 | 0.419 | 4.946 |
| 6 | -0.454 | -0.618 | 4.307 |
| 8 | 1.376 | -1.762 | 1.181 |
| 8 | -0.004 | 1.403 | 1.960 |
| 24 | 0.843 | 3.108 | 2.167 |
| 8 | 1.882 | 4.848 | 2.241 |
| 8 | 2.415 | 2.191 | 1.561 |
| 6 | -1.064 | -1.469 | 5.412 |
| 8 | -1.689 | -0.542 | 6.290 |
| 8 | 0.118 | -2.789 | 3.319 |
| 8 | 0.247 | 3.708 | 0.325 |
| 8 | -0.786 | 4.138 | 2.808 |
| 8 | 1.151 | 2.663 | 4.063 |
| 1 | -1.825 | -0.955 | 7.149 |
| 1 | -1.263 | -0.154 | 3.728 |
| 1 | -0.281 | -2.028 | 5.939 |
| 1 | -1.787 | -2.173 | 4.989 |
| 1 | 0.631 | -3.303 | 3.952 |
| 1 | 1.508 | -1.319 | 3.788 |
| 1 | -0.552 | -1.076 | 1.543 |
| 1 | 3.052 | 0.214 | 1.402 |
| 1 | 1.416 | 0.482 | 0.509 |
| 1 | 1.221 | -2.680 | 1.448 |
| 1 | 0.812 | 1.756 | 4.373 |
| 1 | 2.017 | 2.823 | 4.463 |
| 1 | 1.579 | 5.590 | 2.783 |
| 1 | 2.849 | 4.836 | 2.259 |
| 1 | 0.797 | 4.338 | -0.161 |
| 1 | -0.107 | 3.071 | -0.311 |
| 1 | -1.179 | 3.940 | 3.669 |
| 1 | -1.503 | 4.327 | 2.186 |
| 1 | -0.190 | 0.621 | 5.762 |

$[Cr(H_2O)_4]^{3+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -1.835 | -1.726 | 1.351 |
| 6 | -2.630 | -0.906 | 2.230 |
| 6 | -2.411 | 0.559 | 1.909 |
| 6 | -2.772 | 0.972 | 0.474 |
| 6 | -1.492 | 1.655 | -0.026 |
| 6 | -0.412 | 0.995 | 0.840 |
| 8 | -0.997 | 0.854 | 2.071 |
| 6 | 0.939 | 1.676 | 0.998 |
| 8 | 1.777 | 1.292 | -0.119 |
| 24 | 1.536 | -0.608 | -0.694 |
| 8 | -3.896 | 1.812 | 0.505 |
| 8 | -1.270 | 1.496 | -1.414 |
| 8 | -0.101 | -0.329 | 0.293 |
| 8 | 0.534 | -0.109 | -2.297 |
| 8 | 1.191 | -2.490 | -1.208 |
| 8 | 2.492 | -1.183 | 0.956 |
| 8 | 3.290 | -0.778 | -1.628 |
| 1 | -2.388 | -2.301 | 0.808 |
| 1 | -3.688 | -1.157 | 2.123 |
| 1 | -2.312 | -1.116 | 3.254 |
| 1 | -4.312 | 1.820 | -0.365 |
| 1 | -1.387 | 2.334 | -1.877 |
| 1 | -0.223 | 0.520 | -2.074 |
| 1 | -1.534 | 2.718 | 0.235 |
| 1 | 0.861 | 2.762 | 1.033 |
| 1 | 1.855 | 2.004 | -0.772 |
| 1 | 1.425 | 1.306 | 1.902 |
| 1 | -0.786 | -1.034 | 0.675 |
| 1 | 0.480 | -2.676 | -1.840 |
| 1 | 1.251 | -3.230 | -0.586 |
| 1 | 3.440 | -1.506 | -2.250 |
| 1 | 3.416 | -1.473 | 0.922 |
| 1 | 2.064 | -1.589 | 1.724 |
| 1 | 3.848 | -0.031 | -1.893 |
| 1 | -2.962 | 0.093 | -0.154 |
| 1 | -2.957 | 1.177 | 2.626 |
| 1 | 0.976 | 0.181 | -3.109 |

$[Cr(H_2O)_6]^{3+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.482 | -1.818 | 0.976 |
| 6 | 0.346 | -0.997 | 1.968 |
| 8 | -0.417 | -0.677 | 3.085 |
| 6 | -1.614 | 0.066 | 2.821 |
| 6 | -2.529 | -0.754 | 1.916 |
| 6 | -1.797 | -1.134 | 0.634 |
| 8 | 0.852 | 0.170 | 1.327 |
| 6 | -2.253 | 0.373 | 4.155 |
| 8 | -1.441 | 1.316 | 4.833 |
| 8 | -3.674 | 0.014 | 1.621 |
| 8 | -2.661 | -1.990 | -0.084 |
| 8 | 0.231 | -2.106 | -0.224 |
| 8 | 0.785 | 1.407 | -0.883 |
| 24 | 1.683 | 0.828 | -2.511 |
| 8 | 2.673 | 0.376 | -4.173 |
| 8 | 2.419 | 2.664 | -2.679 |
| 8 | 0.856 | -0.926 | -2.389 |
| 8 | 0.187 | 1.384 | -3.684 |
| 8 | 3.294 | 0.214 | -1.528 |
| 1 | -1.851 | 1.516 | 5.681 |
| 1 | -2.345 | -0.558 | 4.730 |
| 1 | -3.257 | 0.773 | 3.969 |
| 1 | -1.357 | 1.011 | 2.324 |
| 1 | -2.811 | -1.683 | 2.439 |
| 1 | -4.192 | -0.482 | 0.973 |
| 1 | -1.618 | -0.213 | 0.061 |
| 1 | -2.358 | -2.060 | -0.997 |
| 1 | -0.716 | -2.764 | 1.475 |
| 1 | 0.787 | -2.886 | -0.107 |
| 1 | 1.190 | -1.584 | 2.342 |
| 1 | 3.874 | 0.832 | -1.059 |
| 1 | 0.000 | 1.970 | -0.928 |
| 1 | 2.436 | 3.296 | -1.945 |
| 1 | 0.013 | 2.313 | -3.899 |
| 1 | 3.475 | -0.168 | -4.170 |
| 1 | 0.570 | -1.361 | -1.514 |
| 1 | -0.649 | 0.896 | -3.686 |
| 1 | 1.075 | -1.617 | -3.031 |
| 1 | 2.231 | 0.287 | -5.030 |
| 1 | 3.326 | -0.638 | -1.067 |
| 1 | 0.778 | 0.888 | -0.009 |
| 1 | 3.123 | 2.884 | -3.307 |
| 1 | 1.490 | 0.599 | 1.913 |

$[Cr(H_2O)_6]^{3+}$-TS2

| | | | |
|---|---|---|---|
| 6 | -0.200 | -0.412 | 2.292 |
| 8 | 0.323 | -0.702 | 1.127 |
| 6 | -0.124 | -1.161 | 3.486 |
| 6 | -0.938 | -0.749 | 4.708 |
| 6 | -0.106 | -0.855 | 5.999 |
| 6 | -0.937 | -0.512 | 7.233 |
| 8 | -2.040 | -1.403 | 7.294 |
| 8 | 0.575 | -2.270 | 3.548 |
| 8 | -2.036 | -1.623 | 4.662 |
| 8 | 0.422 | -2.189 | 6.045 |
| 6 | -0.155 | -0.585 | 8.540 |
| 8 | -1.043 | -0.394 | 9.628 |
| 8 | 1.686 | -2.764 | 0.630 |
| 24 | 1.113 | -4.483 | 0.245 |
| 8 | -0.630 | -3.820 | -0.497 |
| 8 | 0.369 | -4.617 | 2.069 |
| 8 | 1.973 | -4.408 | -1.549 |
| 8 | 0.455 | -6.343 | -0.267 |
| 8 | 2.754 | -5.406 | 0.913 |
| 1 | -1.295 | 0.521 | 7.094 |
| 1 | -0.910 | 0.415 | 2.290 |
| 1 | -1.201 | 0.550 | 9.748 |
| 1 | 0.660 | 0.148 | 8.544 |
| 1 | 0.265 | -1.587 | 8.670 |
| 1 | 1.224 | -2.218 | 6.583 |
| 1 | 0.714 | -0.129 | 5.933 |
| 1 | -1.242 | 0.302 | 4.597 |
| 1 | 0.673 | -2.490 | 4.537 |
| 1 | -2.480 | -1.263 | 8.145 |
| 1 | -2.388 | -1.693 | 5.572 |
| 1 | 2.262 | -3.561 | -1.917 |
| 1 | 1.728 | -5.003 | -2.271 |
| 1 | 0.842 | -7.145 | 0.109 |
| 1 | -0.466 | -6.527 | -0.500 |
| 1 | 3.576 | -5.379 | 0.403 |
| 1 | -1.343 | -3.568 | 0.108 |
| 1 | 2.975 | -5.392 | 1.856 |
| 1 | -0.632 | -3.181 | -1.226 |
| 1 | 0.344 | -3.801 | 2.610 |
| 1 | 2.596 | -2.680 | 0.942 |
| 1 | 0.869 | -1.565 | 1.043 |
| 1 | -0.306 | -5.241 | 2.367 |
| 1 | 0.632 | 0.010 | 3.178 |

$[Cr(H_2O)_6]^{3+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.157 | 1.109 | -3.729 |
| 6 | 1.114 | 1.680 | -3.829 |
| 6 | 1.294 | 1.823 | -5.354 |
| 6 | 0.642 | 0.559 | -5.902 |
| 6 | -0.420 | 0.225 | -4.839 |
| 6 | 1.014 | 2.951 | -2.992 |
| 8 | 2.294 | 3.520 | -2.730 |
| 8 | 2.086 | 0.813 | -3.255 |
| 8 | 2.646 | 1.951 | -5.764 |

| | | | |
|---|---|---|---|
| 8 | 0.119 | 0.831 | -7.182 |
| 6 | -0.390 | -1.207 | -4.350 |
| 8 | 0.936 | -1.489 | -3.900 |
| 8 | 4.287 | 3.219 | -4.269 |
| 24 | 5.780 | 2.261 | -3.514 |
| 8 | 5.547 | 3.089 | -1.725 |
| 8 | 6.189 | 1.349 | -5.229 |
| 8 | 4.608 | 0.780 | -3.067 |
| 8 | 6.933 | 3.811 | -3.980 |
| 8 | 7.409 | 1.372 | -2.771 |
| 1 | 0.939 | -2.281 | -3.351 |
| 1 | -1.109 | -1.329 | -3.533 |
| 1 | -0.663 | -1.881 | -5.171 |
| 1 | -1.417 | 0.460 | -5.221 |
| 1 | 1.400 | -0.232 | -5.956 |
| 1 | 0.374 | 3.665 | -3.517 |
| 1 | 3.554 | 3.480 | -3.622 |
| 1 | 3.756 | 2.759 | -4.992 |
| 1 | 0.713 | 2.692 | -5.686 |
| 1 | 2.667 | 2.086 | -6.721 |
| 1 | 0.037 | 0.008 | -7.676 |
| 1 | 6.469 | 1.814 | -6.032 |
| 1 | 5.696 | 0.555 | -5.486 |
| 1 | 1.765 | -0.120 | -3.391 |
| 1 | 5.772 | 4.020 | -1.574 |
| 1 | 4.837 | 2.837 | -1.116 |
| 1 | 4.856 | 0.102 | -2.423 |
| 1 | 7.594 | 1.326 | -1.821 |
| 1 | 7.844 | 0.629 | -3.213 |
| 1 | 3.587 | 0.840 | -3.150 |
| 1 | 7.899 | 3.761 | -4.017 |
| 1 | 6.625 | 4.506 | -4.581 |
| 1 | 0.544 | 2.668 | -2.046 |
| 1 | 2.179 | 4.342 | -2.238 |

$[Cr(H_2O)_3OH]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.091 | 0.743 | 4.603 |
| 6 | -1.122 | 0.479 | 3.501 |
| 6 | -0.424 | -0.235 | 2.351 |
| 6 | 0.240 | -1.504 | 2.842 |
| 6 | 1.097 | -1.278 | 4.081 |
| 8 | 0.491 | -0.506 | 5.030 |
| 8 | -1.629 | 1.687 | 2.973 |
| 8 | -1.304 | -0.635 | 1.326 |
| 8 | 1.100 | -2.046 | 1.821 |
| 24 | 3.102 | -1.475 | 1.915 |
| 8 | 4.834 | -1.157 | 2.349 |
| 8 | 2.323 | -0.654 | 3.581 |
| 6 | -0.687 | 1.383 | 5.833 |
| 8 | 0.369 | 1.784 | 6.684 |
| 8 | 2.757 | 0.279 | 0.991 |
| 8 | 3.374 | -3.218 | 2.881 |
| 8 | 3.680 | -2.161 | 0.116 |
| 1 | -0.010 | 2.191 | 7.470 |
| 1 | 0.702 | 1.394 | 4.211 |
| 1 | -1.350 | 0.662 | 6.329 |
| 1 | -1.285 | 2.246 | 5.513 |
| 1 | -2.505 | 1.860 | 3.334 |
| 1 | -1.930 | -0.155 | 3.889 |
| 1 | 0.339 | 0.448 | 1.949 |
| 1 | 1.375 | -2.218 | 4.561 |
| 1 | -0.522 | -2.252 | 3.079 |
| 1 | -1.666 | 0.159 | 0.912 |
| 1 | 0.593 | -2.116 | 0.996 |
| 1 | 5.215 | -0.305 | 2.103 |
| 1 | 4.307 | -3.401 | 3.065 |
| 1 | 2.953 | -4.039 | 2.590 |
| 1 | 2.949 | -0.512 | 4.311 |
| 1 | 2.946 | 1.115 | 1.441 |
| 1 | 3.050 | 0.366 | 0.072 |
| 1 | 4.637 | -2.303 | 0.065 |
| 1 | 3.247 | -2.887 | -0.355 |

$[Cr(H_2O)_3OH]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.138 | 0.925 | 1.201 |
| 6 | 0.963 | 0.493 | 1.857 |
| 6 | 0.513 | -0.936 | 2.024 |
| 6 | 0.296 | -1.255 | 3.542 |
| 6 | -1.128 | -0.933 | 4.002 |
| 8 | -1.556 | 0.334 | 3.459 |
| 8 | 2.448 | 2.197 | 1.230 |
| 24 | 1.328 | 3.305 | 2.338 |
| 8 | 2.242 | 4.870 | 2.138 |
| 8 | 0.114 | 3.967 | 0.858 |
| 8 | 0.250 | 1.467 | 2.397 |
| 8 | 0.197 | 4.319 | 3.714 |
| 8 | 2.373 | 2.620 | 3.935 |
| 8 | 1.498 | -1.749 | 1.469 |
| 8 | 0.470 | -2.646 | 3.688 |
| 6 | -1.267 | -0.861 | 5.513 |
| 8 | -2.557 | -0.313 | 5.738 |
| 1 | -2.609 | 0.034 | 6.636 |
| 1 | -1.798 | -1.698 | 3.594 |
| 1 | -0.489 | -0.210 | 5.932 |
| 1 | -1.169 | -1.864 | 5.942 |
| 1 | 1.177 | -2.825 | 4.318 |
| 1 | 1.034 | -0.708 | 4.140 |
| 1 | -0.448 | -1.065 | 1.501 |
| 1 | 2.856 | 0.189 | 0.840 |
| 1 | 1.131 | 0.646 | 0.445 |
| 1 | 1.392 | -2.622 | 1.881 |
| 1 | 3.335 | 2.577 | 3.841 |
| 1 | 3.141 | 4.778 | 1.800 |
| 1 | 0.533 | 4.719 | 0.413 |
| 1 | -0.305 | 3.414 | 0.184 |
| 1 | 0.446 | 5.255 | 3.732 |
| 1 | -0.769 | 4.275 | 3.717 |
| 1 | -2.191 | 0.719 | 4.096 |
| 1 | -0.650 | 1.070 | 2.922 |
| 1 | 2.188 | 3.056 | 4.779 |

$[Cr(H_2O)_3OH]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.788 | 0.631 | 1.903 |
| 6 | -2.219 | 0.431 | 1.796 |
| 6 | -2.615 | 0.907 | 0.389 |
| 6 | -1.323 | 1.543 | -0.136 |
| 6 | -0.240 | 0.785 | 0.646 |
| 6 | -2.537 | -1.021 | 2.082 |
| 1 | -2.133 | -1.298 | 3.060 |
| 8 | -3.696 | 1.802 | 0.490 |
| 8 | -1.181 | 1.451 | -1.541 |
| 6 | 1.125 | 1.439 | 0.798 |
| 8 | 1.884 | 1.092 | -0.374 |
| 24 | 1.678 | -0.784 | -1.093 |
| 8 | 3.277 | -0.636 | -1.950 |
| 8 | 0.003 | -0.504 | 0.042 |
| 8 | 0.621 | -0.106 | -2.631 |
| 8 | 1.146 | -2.623 | -1.689 |
| 8 | 2.641 | -1.689 | 0.434 |
| 8 | -1.943 | -1.817 | 1.051 |
| 1 | -3.623 | -1.163 | 2.082 |
| 1 | -4.136 | 1.861 | -0.365 |
| 1 | -1.278 | 2.323 | -1.941 |
| 1 | -0.103 | 0.508 | -2.322 |
| 1 | -1.297 | 2.590 | 0.182 |
| 1 | 1.042 | 2.525 | 0.863 |
| 1 | 2.772 | 1.479 | -0.358 |
| 1 | 1.613 | 1.045 | 1.694 |
| 1 | -0.682 | -1.168 | 0.383 |
| 1 | 0.818 | -2.735 | -2.593 |
| 1 | 1.715 | -3.377 | -1.479 |
| 1 | 3.492 | -1.284 | -2.631 |
| 1 | 3.602 | -1.576 | 0.439 |
| 1 | 2.326 | -1.733 | 1.346 |
| 1 | -2.876 | 0.058 | -0.254 |
| 1 | -2.696 | 1.062 | 2.550 |
| 1 | 1.143 | 0.344 | -3.309 |
| 1 | -1.897 | -2.741 | 1.324 |

$[Cr(H_2O)_3Cl]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 8 | -0.037 | 0.737 | 4.562 |
| 6 | -1.055 | 0.412 | 3.589 |
| 6 | -0.412 | -0.285 | 2.385 |
| 6 | 0.642 | 0.647 | 1.803 |
| 6 | 1.658 | 1.018 | 2.861 |
| 6 | 1.014 | 1.498 | 4.155 |
| 6 | -2.071 | -0.447 | 4.300 |
| 8 | -2.763 | 0.360 | 5.234 |
| 8 | -1.359 | -0.505 | 1.361 |
| 8 | 1.383 | 0.075 | 0.752 |
| 8 | 2.508 | 2.086 | 2.382 |
| 24 | 1.941 | 3.983 | 2.884 |
| 8 | 3.239 | 4.914 | 1.678 |
| 8 | 0.598 | 2.881 | 3.866 |
| 17 | 1.231 | 5.902 | 3.753 |
| 8 | 0.644 | 4.051 | 1.357 |
| 8 | 3.232 | 3.767 | 4.396 |
| 1 | -3.410 | -0.189 | 5.691 |
| 1 | -1.541 | 1.339 | 3.256 |
| 1 | -1.555 | -1.281 | 4.795 |
| 1 | -2.757 | -0.855 | 3.547 |
| 1 | -1.620 | -1.432 | 1.351 |
| 1 | 0.056 | -1.226 | 2.703 |
| 1 | 0.127 | 1.555 | 1.456 |
| 1 | 1.727 | 1.537 | 4.981 |
| 1 | 2.300 | 0.161 | 3.085 |
| 1 | 0.789 | -0.065 | 0.003 |
| 1 | 2.837 | 1.844 | 1.499 |
| 1 | 3.386 | 4.534 | 4.967 |
| 1 | 4.076 | 3.309 | 4.265 |
| 1 | 0.186 | 3.278 | 4.652 |
| 1 | -0.228 | 4.441 | 1.528 |
| 1 | 0.973 | 4.440 | 0.532 |
| 1 | 3.328 | 5.872 | 1.803 |
| 1 | 4.117 | 4.564 | 1.464 |

$[Cr(H_2O)_3Cl]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 1.998 | 0.788 | 1.361 |
| 8 | 2.299 | 2.061 | 1.355 |
| 24 | 0.830 | 3.227 | 1.765 |
| 8 | 1.164 | 3.217 | 3.753 |
| 6 | 0.658 | 0.430 | 1.640 |
| 8 | -0.155 | 1.453 | 1.823 |
| 6 | 0.151 | -0.988 | 1.775 |
| 8 | 1.261 | -1.820 | 1.617 |
| 6 | -0.558 | -1.278 | 3.131 |
| 8 | -0.666 | -2.684 | 3.171 |

| | | | |
|---|---|---|---|
| 6 | -1.977 | -0.715 | 3.201 |
| 6 | -2.803 | -1.163 | 4.388 |
| 8 | -3.968 | -0.355 | 4.322 |
| 8 | -1.884 | 0.739 | 3.342 |
| 8 | -0.914 | 4.177 | 2.238 |
| 8 | 0.235 | 3.447 | -0.148 |
| 17 | 2.045 | 5.118 | 1.602 |
| 1 | -4.400 | -0.336 | 5.183 |
| 1 | -2.522 | -0.921 | 2.273 |
| 1 | -2.253 | -0.995 | 5.322 |
| 1 | -3.037 | -2.226 | 4.287 |
| 1 | -0.360 | -3.015 | 4.023 |
| 1 | 0.045 | -0.897 | 3.963 |
| 1 | -0.590 | -1.162 | 0.978 |
| 1 | 2.782 | 0.034 | 1.300 |
| 1 | 1.240 | 0.420 | 0.361 |
| 1 | 0.965 | -2.717 | 1.832 |
| 1 | 1.894 | 3.786 | 4.038 |
| 1 | 1.199 | 2.408 | 4.283 |
| 1 | -1.281 | 4.784 | 1.580 |
| 1 | -0.957 | 4.622 | 3.096 |
| 1 | -2.786 | 1.102 | 3.460 |
| 1 | -1.256 | 1.178 | 2.601 |
| 1 | -0.258 | 2.765 | -0.625 |
| 1 | 0.850 | 3.866 | -0.766 |

$[Cr(H_2O)_3Cl]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.788 | 0.631 | 1.903 |
| 6 | -2.219 | 0.431 | 1.796 |
| 6 | -2.615 | 0.907 | 0.389 |
| 6 | -1.323 | 1.543 | -0.136 |
| 6 | -0.240 | 0.785 | 0.646 |
| 6 | -2.537 | -1.021 | 2.082 |
| 1 | -2.133 | -1.298 | 3.060 |
| 8 | -3.696 | 1.802 | 0.490 |
| 8 | -1.181 | 1.451 | -1.541 |
| 6 | 1.125 | 1.439 | 0.798 |
| 8 | 1.884 | 1.092 | -0.374 |
| 24 | 1.678 | -0.784 | -1.093 |
| 8 | 3.277 | -0.636 | -1.950 |
| 8 | 0.003 | -0.504 | 0.042 |
| 8 | 0.621 | -0.106 | -2.631 |
| 8 | 1.146 | -2.623 | -1.689 |
| 8 | 2.641 | -1.689 | 0.434 |
| 8 | -1.943 | -1.817 | 1.051 |
| 1 | -3.623 | -1.163 | 2.082 |
| 1 | -4.136 | 1.861 | -0.365 |
| 1 | -1.278 | 2.323 | -1.941 |
| 1 | -0.103 | 0.508 | -2.322 |
| 1 | -1.297 | 2.590 | 0.182 |
| 1 | 1.042 | 2.525 | 0.863 |
| 1 | 2.772 | 1.479 | -0.358 |
| 1 | 1.613 | 1.045 | 1.694 |
| 1 | -0.682 | -1.168 | 0.383 |
| 1 | 0.818 | -2.735 | -2.593 |
| 1 | 1.715 | -3.377 | -1.479 |
| 1 | 3.492 | -1.284 | -2.631 |
| 1 | 3.602 | -1.576 | 0.439 |
| 1 | 2.326 | -1.733 | 1.346 |
| 1 | -2.876 | 0.058 | -0.254 |
| 1 | -2.696 | 1.062 | 2.550 |
| 1 | 1.143 | 0.344 | -3.309 |
| 1 | -1.897 | -2.741 | 1.324 |

$[Cr(H_2O)_2Cl_2]^{+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.049 | 0.733 | 4.562 |
| 8 | -1.017 | 0.408 | 3.652 |
| 6 | -0.592 | -0.235 | 2.434 |
| 6 | 0.169 | -1.522 | 2.771 |
| 6 | 1.354 | -1.164 | 3.658 |
| 6 | 0.882 | -0.427 | 4.894 |
| 6 | -1.837 | -0.480 | 1.617 |
| 8 | -2.330 | 0.768 | 1.167 |
| 8 | 0.708 | -2.118 | 1.608 |
| 8 | 2.061 | -2.290 | 4.125 |
| 8 | 2.000 | 0.128 | 5.613 |
| 24 | 2.557 | 2.048 | 5.144 |
| 8 | 1.444 | 2.547 | 6.753 |
| 8 | 0.829 | 1.785 | 4.064 |
| 17 | 4.455 | 1.853 | 6.333 |
| 17 | 2.668 | 4.216 | 4.557 |
| 8 | 3.544 | 1.444 | 3.489 |
| 1 | -3.126 | 0.612 | 0.648 |
| 1 | 0.071 | 0.443 | 1.880 |
| 1 | -2.578 | -1.002 | 2.238 |
| 1 | -1.570 | -1.126 | 0.772 |
| 1 | 0.164 | -2.864 | 1.339 |
| 1 | -0.492 | -2.220 | 3.303 |
| 1 | 2.021 | -0.511 | 3.077 |
| 1 | -0.559 | 1.110 | 5.451 |
| 1 | 0.359 | -1.117 | 5.563 |
| 1 | 2.465 | -2.726 | 3.364 |
| 1 | 2.673 | -0.557 | 5.758 |
| 1 | 1.416 | 3.498 | 6.937 |
| 1 | 1.670 | 2.099 | 7.582 |
| 1 | 0.316 | 2.586 | 3.868 |
| 1 | 3.414 | 1.989 | 2.699 |
| 1 | 4.501 | 1.362 | 3.622 |

$[Cr(H_2O)_2Cl_2]^{+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.059 | 0.764 | 1.306 |
| 8 | 3.042 | -0.064 | 1.064 |
| 24 | 4.752 | 0.788 | 0.632 |
| 8 | 4.277 | 0.839 | -1.340 |
| 6 | 2.322 | 2.154 | 1.247 |
| 8 | 3.545 | 2.460 | 0.867 |
| 6 | 1.335 | 3.244 | 1.595 |
| 8 | 0.188 | 2.606 | 2.072 |
| 6 | 1.870 | 4.265 | 2.645 |
| 8 | 0.721 | 4.974 | 3.056 |
| 6 | 2.848 | 5.281 | 2.051 |
| 6 | 3.231 | 6.416 | 2.976 |
| 8 | 4.242 | 7.120 | 2.272 |
| 8 | 4.086 | 4.586 | 1.743 |
| 17 | 5.787 | -1.203 | 0.303 |
| 8 | 5.214 | 0.786 | 2.602 |
| 17 | 6.544 | 2.182 | 0.288 |
| 1 | 4.743 | 7.667 | 2.886 |
| 1 | 2.445 | 5.691 | 1.117 |
| 1 | 3.611 | 6.018 | 3.925 |
| 1 | 2.356 | 7.044 | 3.167 |
| 1 | 0.675 | 4.997 | 4.018 |
| 1 | 2.335 | 3.734 | 3.484 |
| 1 | 1.117 | 3.812 | 0.675 |
| 1 | 1.115 | 0.402 | 1.713 |
| 1 | 1.628 | 1.394 | 0.258 |
| 1 | -0.385 | 3.303 | 2.424 |
| 1 | 4.567 | 0.478 | 3.251 |
| 1 | 5.669 | 1.560 | 2.961 |
| 1 | 4.737 | 5.226 | 1.400 |
| 1 | 3.919 | 3.589 | 1.192 |
| 1 | 4.004 | 1.675 | -1.743 |
| 1 | 3.701 | 0.140 | -1.680 |

$[Cr(H_2O)_2Cl_2]^{+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.558 | 1.953 | 1.134 |
| 6 | -0.782 | 0.632 | 1.884 |
| 8 | -2.138 | 0.408 | 1.766 |
| 6 | -2.600 | 0.875 | 0.474 |
| 6 | -1.503 | 1.809 | -0.062 |
| 6 | -0.393 | 0.565 | 3.350 |
| 8 | 1.021 | 0.307 | 3.372 |
| 24 | 1.636 | -1.158 | 2.057 |
| 8 | 0.544 | -2.469 | 3.168 |
| 8 | -0.043 | -0.430 | 1.235 |
| 6 | -2.895 | -0.321 | -0.404 |
| 8 | -1.663 | -1.012 | -0.644 |
| 8 | -2.088 | 3.018 | -0.482 |
| 8 | 0.787 | 2.179 | 0.758 |
| 17 | 3.472 | -1.593 | 3.306 |
| 8 | 2.589 | 0.258 | 1.021 |
| 17 | 1.896 | -2.706 | 0.432 |
| 1 | -3.610 | -0.979 | 0.099 |
| 1 | -3.320 | 0.020 | -1.354 |
| 1 | -1.471 | 3.478 | -1.062 |
| 1 | 1.081 | 3.037 | 1.085 |
| 1 | 1.991 | 1.040 | 0.878 |
| 1 | -0.921 | 2.767 | 1.770 |
| 1 | -0.599 | 1.507 | 3.860 |
| 1 | 1.363 | 0.288 | 4.277 |
| 1 | -0.934 | -0.257 | 3.826 |
| 1 | -0.590 | -0.816 | 0.473 |
| 1 | 1.068 | -2.902 | 3.858 |
| 1 | 0.129 | -3.176 | 2.651 |
| 1 | -0.956 | 1.338 | -0.888 |
| 1 | -3.521 | 1.440 | 0.640 |
| 1 | 3.418 | 0.567 | 1.413 |
| 1 | -1.834 | -1.904 | -0.966 |

$[Cr_2(H_2O)_7OH]^{5+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | 2.076 | 0.929 | 1.520 |
| 8 | 2.228 | 2.220 | 1.621 |
| 24 | 0.524 | 3.162 | 2.081 |
| 8 | 0.154 | 3.459 | 0.134 |
| 6 | 0.734 | 0.486 | 1.643 |
| 8 | -0.184 | 1.400 | 1.933 |
| 6 | 0.377 | -0.969 | 1.859 |
| 8 | 1.254 | -1.722 | 1.064 |
| 6 | 0.494 | -1.402 | 3.330 |
| 8 | 0.070 | -2.754 | 3.291 |
| 6 | -0.333 | -0.572 | 4.326 |
| 6 | -0.778 | -1.405 | 5.523 |
| 8 | -1.208 | -0.461 | 6.495 |
| 8 | 0.497 | 0.486 | 4.845 |
| 24 | 3.543 | 3.727 | 1.752 |
| 8 | 3.636 | 3.370 | 3.700 |
| 8 | 3.538 | 3.953 | -0.228 |
| 8 | 1.851 | 4.629 | 1.937 |
| 8 | 4.659 | 5.340 | 1.970 |
| 8 | 5.267 | 2.710 | 1.638 |
| 8 | -1.189 | 4.004 | 2.676 |
| 8 | 0.960 | 2.797 | 4.001 |
| 1 | -1.199 | -0.871 | 7.367 |
| 1 | -1.211 | -0.123 | 3.847 |
| 1 | 0.062 | -1.994 | 5.911 |
| 1 | -1.587 | -2.079 | 5.230 |

| | | | |
|---|---|---|---|
| 1 | 0.627 | -3.290 | 3.865 |
| 1 | 1.547 | -1.334 | 3.632 |
| 1 | -0.669 | -1.091 | 1.544 |
| 1 | 2.918 | 0.274 | 1.307 |
| 1 | 1.117 | 0.523 | 0.447 |
| 1 | 1.122 | -2.651 | 1.302 |
| 1 | 0.715 | 1.828 | 4.310 |
| 1 | 0.530 | 3.409 | 4.620 |
| 1 | 1.773 | 5.444 | 2.452 |
| 1 | 0.303 | 4.340 | -0.240 |
| 1 | -0.652 | 3.096 | -0.262 |
| 1 | -1.987 | 3.455 | 2.709 |
| 1 | -1.452 | 4.885 | 2.371 |
| 1 | 0.174 | 0.613 | 5.761 |
| 1 | 5.525 | 2.115 | 2.358 |
| 1 | 3.427 | 3.240 | -0.874 |
| 1 | 2.768 | 3.143 | 4.104 |
| 1 | 5.618 | 5.299 | 1.839 |
| 1 | 4.075 | 4.023 | 4.267 |
| 1 | 4.362 | 6.254 | 1.849 |
| 1 | 3.968 | 4.702 | -0.665 |
| 1 | 5.627 | 2.359 | 0.810 |

$[Cr(H_2O)Cl_3]$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | 0.880 | -0.370 | 4.866 |
| 6 | -0.060 | 0.776 | 4.517 |
| 8 | -1.042 | 0.406 | 3.631 |
| 6 | -0.620 | -0.246 | 2.419 |
| 6 | 0.178 | -1.509 | 2.763 |
| 6 | 1.360 | -1.109 | 3.635 |
| 8 | 0.792 | 1.818 | 3.980 |
| 24 | 2.512 | 2.108 | 5.148 |
| 17 | 3.790 | 1.539 | 3.305 |
| 6 | -1.870 | -0.537 | 1.625 |
| 8 | -2.402 | 0.689 | 1.159 |
| 8 | 0.721 | -2.102 | 1.599 |
| 8 | 2.103 | -2.211 | 4.110 |
| 8 | 1.995 | 0.190 | 5.588 |
| 17 | 1.099 | 2.962 | 6.782 |
| 17 | 4.303 | 2.050 | 6.539 |
| 8 | 2.715 | 4.016 | 4.533 |
| 1 | -3.200 | 0.502 | 0.652 |
| 1 | 0.020 | 0.438 | 1.844 |
| 1 | -2.588 | -1.066 | 2.266 |
| 1 | -1.599 | -1.192 | 0.787 |
| 1 | 0.196 | -2.868 | 1.347 |
| 1 | -0.459 | -2.218 | 3.307 |
| 1 | 2.005 | -0.443 | 3.045 |
| 1 | -0.563 | 1.167 | 5.405 |
| 1 | 0.360 | -1.060 | 5.538 |
| 1 | 2.540 | -2.624 | 3.355 |
| 1 | 2.712 | -0.465 | 5.624 |
| 1 | 0.264 | 2.623 | 3.862 |
| 1 | 3.511 | 4.194 | 4.011 |
| 1 | 2.644 | 4.687 | 5.228 |

$[Cr(H_2O)Cl_3]$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.065 | 0.768 | 1.320 |
| 6 | 2.338 | 2.158 | 1.302 |
| 6 | 1.334 | 3.273 | 1.426 |
| 6 | 1.786 | 4.286 | 2.532 |
| 6 | 2.695 | 5.388 | 1.981 |
| 8 | 3.667 | 4.834 | 1.072 |
| 8 | 3.068 | -0.070 | 1.301 |
| 24 | 4.784 | 0.779 | 0.849 |
| 17 | 6.647 | 2.046 | 0.309 |
| 17 | 4.060 | 0.753 | -1.378 |
| 8 | 3.611 | 2.454 | 1.153 |
| 8 | 5.686 | -0.996 | 0.523 |
| 17 | 5.440 | 0.616 | 3.073 |
| 8 | 0.104 | 2.696 | 1.741 |
| 8 | 0.616 | 4.920 | 2.999 |
| 6 | 3.446 | 6.137 | 3.068 |
| 8 | 4.387 | 6.945 | 2.378 |
| 1 | 5.082 | 7.221 | 2.986 |
| 1 | 2.073 | 6.082 | 1.404 |
| 1 | 3.956 | 5.426 | 3.730 |
| 1 | 2.744 | 6.739 | 3.656 |
| 1 | 0.515 | 4.765 | 3.945 |
| 1 | 2.279 | 3.741 | 3.345 |
| 1 | 1.284 | 3.811 | 0.465 |
| 1 | 1.066 | 0.434 | 1.602 |
| 1 | 1.853 | 1.295 | 0.184 |
| 1 | -0.430 | 3.403 | 2.139 |
| 1 | 4.459 | 5.405 | 1.112 |
| 1 | 3.791 | 3.540 | 1.075 |
| 1 | 5.958 | -1.124 | -0.397 |
| 1 | 6.461 | -1.141 | 1.084 |

$[Cr(H_2O)Cl_3]$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.238 | 0.889 | 0.593 |
| 8 | -0.718 | 0.564 | 1.847 |
| 6 | -2.151 | 0.352 | 1.777 |
| 6 | -2.605 | 0.941 | 0.433 |
| 6 | -1.365 | 1.713 | -0.040 |
| 6 | -2.431 | -1.123 | 1.956 |
| 8 | -1.843 | -1.826 | 0.856 |
| 8 | -3.741 | 1.747 | 0.645 |
| 8 | -1.272 | 1.945 | -1.413 |
| 6 | 1.134 | 1.527 | 0.743 |
| 8 | 1.853 | 1.278 | -0.476 |
| 24 | 1.659 | -0.687 | -1.139 |
| 8 | 3.464 | -0.672 | -2.054 |
| 8 | -0.053 | -0.319 | -0.193 |
| 17 | 0.817 | 0.147 | -3.151 |
| 17 | 1.086 | -2.824 | -1.668 |
| 17 | 2.812 | -1.346 | 0.763 |
| 1 | -2.001 | -1.466 | 2.902 |
| 1 | -3.514 | -1.291 | 1.969 |
| 1 | -4.128 | 1.964 | -0.211 |
| 1 | -0.894 | 1.169 | -1.862 |
| 1 | -1.376 | 2.692 | 0.455 |
| 1 | 1.048 | 2.605 | 0.897 |
| 1 | 2.760 | 1.606 | -0.392 |
| 1 | 1.651 | 1.056 | 1.583 |
| 1 | -0.649 | -1.049 | 0.173 |
| 1 | -2.831 | 0.146 | -0.289 |
| 1 | -2.609 | 0.910 | 2.599 |
| 1 | -1.717 | -2.755 | 1.080 |
| 1 | 4.110 | -1.299 | -1.699 |
| 1 | 3.438 | -0.769 | -3.017 |

$[Fe(H_2O)_4]^{3+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.024 | 0.766 | 4.556 |
| 6 | -1.067 | 0.531 | 3.467 |
| 6 | -0.460 | -0.259 | 2.329 |
| 6 | 0.877 | 0.299 | 1.860 |
| 8 | 1.711 | 0.680 | 2.858 |
| 6 | 1.175 | 1.486 | 3.933 |
| 8 | -2.175 | -0.206 | 3.913 |
| 8 | -1.328 | -0.228 | 1.169 |
| 26 | -1.048 | 1.131 | -0.283 |
| 8 | -0.449 | 2.555 | -1.552 |
| 8 | 0.501 | 1.447 | 1.002 |
| 6 | 2.308 | 1.711 | 4.903 |
| 8 | 3.258 | 2.557 | 4.284 |
| 8 | -0.649 | 1.571 | 5.532 |
| 8 | 0.004 | -0.236 | -1.333 |
| 8 | -2.582 | 0.645 | -1.467 |
| 8 | -2.266 | 2.465 | 0.611 |
| 1 | 3.984 | 2.703 | 4.900 |
| 1 | 0.853 | 2.454 | 3.527 |
| 1 | 2.749 | 0.742 | 5.175 |
| 1 | 1.893 | 2.174 | 5.806 |
| 1 | -0.429 | 1.249 | 6.413 |
| 1 | 0.293 | -0.197 | 4.977 |
| 1 | -1.380 | 1.521 | 3.101 |
| 1 | 1.421 | -0.406 | 1.229 |
| 1 | -0.331 | -1.306 | 2.617 |
| 1 | -2.613 | 0.303 | 4.608 |
| 1 | -2.163 | -0.696 | 1.340 |
| 1 | -3.073 | 2.269 | 1.111 |
| 1 | -2.306 | 3.389 | 0.322 |
| 1 | -0.911 | 2.709 | -2.391 |
| 1 | 0.209 | 3.255 | -1.432 |
| 1 | 0.545 | -0.029 | -2.109 |
| 1 | -0.065 | -1.199 | -1.243 |
| 1 | -3.482 | 0.999 | -1.404 |
| 1 | -2.568 | -0.075 | -2.115 |
| 1 | 1.312 | 1.908 | 0.730 |

$[Fe(H_2O)_4]^{3+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 0.488 | -1.467 | 3.391 |
| 6 | 0.442 | -1.017 | 1.917 |
| 6 | 0.852 | 0.422 | 1.747 |
| 6 | 2.185 | 0.859 | 1.520 |
| 8 | 0.343 | 0.375 | 4.947 |
| 6 | -0.427 | -0.670 | 4.336 |
| 8 | 1.327 | -1.795 | 1.155 |
| 8 | -0.023 | 1.368 | 1.967 |
| 26 | 0.785 | 3.120 | 2.139 |
| 8 | 2.038 | 4.755 | 2.264 |
| 8 | 2.384 | 2.144 | 1.569 |
| 6 | -0.985 | -1.534 | 5.459 |
| 8 | -1.571 | -0.618 | 6.376 |
| 8 | 0.113 | -2.834 | 3.314 |
| 8 | 0.265 | 3.861 | 0.259 |
| 8 | -0.864 | 4.239 | 2.666 |
| 8 | 0.882 | 2.771 | 4.132 |
| 1 | -1.669 | -1.043 | 7.235 |
| 1 | -1.263 | -0.216 | 3.787 |
| 1 | -0.177 | -2.095 | 5.945 |
| 1 | -1.724 | -2.236 | 5.064 |
| 1 | 0.648 | -3.355 | 3.924 |
| 1 | 1.518 | -1.369 | 3.756 |
| 1 | -0.595 | -1.115 | 1.562 |
| 1 | 3.014 | 0.164 | 1.390 |
| 1 | 1.381 | 0.463 | 0.504 |
| 1 | 1.179 | -2.715 | 1.420 |
| 1 | 0.678 | 1.824 | 4.418 |
| 1 | 1.598 | 3.122 | 4.677 |
| 1 | 1.838 | 5.556 | 2.768 |
| 1 | 2.997 | 4.634 | 2.254 |
| 1 | 0.821 | 4.561 | -0.112 |
| 1 | 0.046 | 3.254 | -0.462 |
| 1 | -1.290 | 4.124 | 3.526 |
| 1 | -1.530 | 4.506 | 2.018 |
| 1 | -0.098 | 0.528 | 5.805 |

$[Fe(H_2O)_4]^{3+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 8 | -1.831 | -1.700 | 1.393 |
| 6 | -2.620 | -0.868 | 2.268 |
| 6 | -2.402 | 0.592 | 1.927 |
| 6 | -2.775 | 0.989 | 0.489 |
| 6 | -1.492 | 1.653 | -0.035 |
| 6 | -0.410 | 1.002 | 0.835 |
| 8 | -0.987 | 0.886 | 2.073 |
| 6 | 0.943 | 1.686 | 0.972 |
| 8 | 1.768 | 1.290 | -0.141 |
| 26 | 1.506 | -0.681 | -0.720 |
| 8 | -3.890 | 1.842 | 0.523 |
| 8 | -1.264 | 1.470 | -1.417 |
| 8 | -0.108 | -0.329 | 0.309 |
| 8 | 0.538 | -0.132 | -2.375 |
| 8 | 1.088 | -2.563 | -1.246 |
| 8 | 2.470 | -1.339 | 0.934 |
| 8 | 3.321 | -0.633 | -1.594 |
| 1 | -2.386 | -2.280 | 0.856 |
| 1 | -3.678 | -1.122 | 2.172 |
| 1 | -2.293 | -1.066 | 3.291 |
| 1 | -4.323 | 1.835 | -0.338 |
| 1 | -1.544 | 2.248 | -1.915 |
| 1 | -0.215 | 0.493 | -2.157 |
| 1 | -1.523 | 2.720 | 0.212 |
| 1 | 0.856 | 2.772 | 1.002 |
| 1 | 1.834 | 1.994 | -0.803 |
| 1 | 1.432 | 1.327 | 1.880 |
| 1 | -0.807 | -1.024 | 0.712 |
| 1 | 0.454 | -2.778 | -1.945 |
| 1 | 1.274 | -3.358 | -0.725 |
| 1 | 3.619 | -1.258 | -2.271 |
| 1 | 3.401 | -1.603 | 0.941 |
| 1 | 2.045 | -1.660 | 1.742 |
| 1 | 3.951 | 0.101 | -1.553 |
| 1 | -2.983 | 0.104 | -0.126 |
| 1 | -2.941 | 1.220 | 2.641 |
| 1 | 0.984 | 0.151 | -3.186 |

$[Fe(H_2O)_6]^{3+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.525 | -1.913 | 0.984 |
| 6 | 0.329 | -1.155 | 2.005 |
| 8 | -0.451 | -0.751 | 3.083 |
| 6 | -1.564 | 0.090 | 2.759 |
| 6 | -2.510 | -0.659 | 1.825 |
| 6 | -1.762 | -1.126 | 0.581 |
| 8 | 0.971 | -0.054 | 1.370 |
| 6 | -2.229 | 0.474 | 4.060 |
| 8 | -1.366 | 1.351 | 4.762 |
| 8 | -3.566 | 0.205 | 1.469 |
| 8 | -2.667 | -1.915 | -0.162 |
| 8 | 0.204 | -2.261 | -0.192 |
| 8 | 0.722 | 1.307 | -0.749 |
| 26 | 1.633 | 0.806 | -2.419 |
| 8 | 2.573 | 0.411 | -4.169 |
| 8 | 2.306 | 2.706 | -2.608 |
| 8 | 1.022 | -1.048 | -2.268 |
| 8 | 0.051 | 1.324 | -3.565 |
| 8 | 3.367 | 0.353 | -1.488 |
| 1 | -1.793 | 1.600 | 5.589 |
| 1 | -2.430 | -0.436 | 4.641 |
| 1 | -3.184 | 0.959 | 3.826 |
| 1 | -1.204 | 1.004 | 2.265 |
| 1 | -2.897 | -1.549 | 2.347 |
| 1 | -4.103 | -0.253 | 0.809 |
| 1 | -1.476 | -0.238 | 0.001 |
| 1 | -2.323 | -2.041 | -1.054 |
| 1 | -0.854 | -2.836 | 1.474 |
| 1 | 0.726 | -3.060 | -0.043 |
| 1 | 1.097 | -1.809 | 2.423 |
| 1 | 3.978 | 1.020 | -1.142 |
| 1 | -0.055 | 1.883 | -0.733 |
| 1 | 2.210 | 3.408 | -1.948 |
| 1 | -0.142 | 2.234 | -3.836 |
| 1 | 3.453 | 0.015 | -4.250 |
| 1 | 0.668 | -1.495 | -1.421 |
| 1 | -0.761 | 0.800 | -3.627 |
| 1 | 1.229 | -1.720 | -2.933 |
| 1 | 2.136 | 0.407 | -5.033 |
| 1 | 3.550 | -0.493 | -1.055 |
| 1 | 0.790 | 0.784 | 0.123 |
| 1 | 2.875 | 3.020 | -3.326 |
| 1 | 1.642 | 0.312 | 1.962 |

$[Fe(H_2O)_6]^{3+}$-TS2

| | | | |
|---|---|---|---|
| 6 | -0.233 | -0.362 | 2.320 |
| 8 | 0.295 | -0.634 | 1.153 |
| 6 | -0.130 | -1.116 | 3.508 |
| 6 | -0.946 | -0.733 | 4.738 |
| 6 | -0.104 | -0.837 | 6.023 |
| 6 | -0.934 | -0.519 | 7.264 |
| 8 | -2.022 | -1.427 | 7.322 |
| 8 | 0.584 | -2.219 | 3.545 |
| 8 | -2.027 | -1.626 | 4.689 |
| 8 | 0.448 | -2.161 | 6.052 |
| 6 | -0.144 | -0.592 | 8.566 |
| 8 | -1.029 | -0.423 | 9.661 |
| 8 | 1.737 | -2.713 | 0.645 |
| 26 | 1.141 | -4.392 | 0.227 |
| 8 | -0.670 | -3.858 | -0.616 |
| 8 | 0.233 | -4.561 | 2.022 |
| 8 | 1.996 | -4.476 | -1.619 |
| 8 | 0.482 | -6.321 | -0.256 |
| 8 | 2.750 | -5.481 | 0.957 |
| 1 | -1.309 | 0.509 | 7.137 |
| 1 | -0.943 | 0.463 | 2.325 |
| 1 | -1.200 | 0.517 | 9.789 |
| 1 | 0.661 | 0.153 | 8.572 |
| 1 | 0.291 | -1.588 | 8.685 |
| 1 | 1.251 | -2.182 | 6.588 |
| 1 | 0.703 | -0.095 | 5.959 |
| 1 | -1.270 | 0.313 | 4.640 |
| 1 | 0.700 | -2.447 | 4.528 |
| 1 | -2.460 | -1.302 | 8.177 |
| 1 | -2.374 | -1.711 | 5.599 |
| 1 | 2.375 | -3.713 | -2.077 |
| 1 | 1.820 | -5.178 | -2.260 |
| 1 | 0.869 | -7.114 | 0.138 |
| 1 | -0.426 | -6.518 | -0.521 |
| 1 | 3.584 | -5.494 | 0.466 |
| 1 | -1.394 | -3.559 | -0.048 |
| 1 | 2.965 | -5.443 | 1.900 |
| 1 | -0.695 | -3.324 | -1.424 |
| 1 | 0.237 | -3.793 | 2.626 |
| 1 | 2.662 | -2.552 | 0.878 |
| 1 | 0.851 | -1.472 | 1.079 |
| 1 | -0.375 | -5.240 | 2.341 |
| 1 | 0.606 | 0.051 | 3.223 |

$[Fe(H_2O)_6]^{3+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.172 | 1.031 | -3.756 |
| 6 | 1.086 | 1.633 | -3.832 |
| 6 | 1.262 | 1.853 | -5.350 |
| 6 | 0.604 | 0.625 | -5.970 |
| 6 | -0.420 | 0.194 | -4.905 |
| 6 | 0.963 | 2.864 | -2.939 |
| 8 | 2.236 | 3.427 | -2.639 |
| 8 | 2.079 | 0.771 | -3.297 |
| 8 | 2.615 | 1.996 | -5.755 |
| 8 | 0.035 | 0.990 | -7.208 |
| 6 | -0.320 | -1.261 | -4.497 |
| 8 | 1.033 | -1.519 | -4.117 |
| 8 | 4.212 | 3.241 | -4.213 |
| 26 | 5.735 | 2.292 | -3.460 |
| 8 | 5.739 | 3.413 | -1.774 |
| 8 | 6.012 | 1.119 | -5.094 |
| 8 | 4.509 | 1.000 | -2.642 |
| 8 | 6.979 | 3.641 | -4.317 |
| 8 | 7.372 | 1.351 | -2.696 |
| 1 | 1.089 | -2.353 | -3.638 |
| 1 | -1.000 | -1.454 | -3.662 |
| 1 | -0.602 | -1.897 | -5.344 |
| 1 | -1.435 | 0.405 | -5.253 |
| 1 | 1.366 | -0.150 | -6.111 |
| 1 | 0.320 | 3.596 | -3.437 |
| 1 | 3.482 | 3.489 | -3.558 |
| 1 | 3.683 | 2.791 | -4.949 |
| 1 | 0.685 | 2.741 | -5.634 |
| 1 | 2.634 | 2.193 | -6.701 |
| 1 | -0.068 | 0.203 | -7.755 |
| 1 | 6.429 | 1.434 | -5.909 |
| 1 | 5.469 | 0.345 | -5.300 |
| 1 | 1.824 | -0.165 | -3.520 |
| 1 | 6.146 | 4.286 | -1.685 |
| 1 | 5.226 | 3.218 | -0.977 |
| 1 | 4.783 | 0.236 | -2.117 |
| 1 | 7.717 | 1.472 | -1.800 |
| 1 | 7.792 | 0.576 | -3.095 |
| 1 | 3.516 | 0.937 | -2.889 |
| 1 | 7.943 | 3.657 | -4.240 |
| 1 | 6.682 | 4.414 | -4.817 |
| 1 | 0.487 | 2.533 | -2.012 |
| 1 | 2.119 | 4.184 | -2.051 |

$[Fe(H_2O)_3Cl]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.015 | 0.756 | 4.560 |
| 6 | -1.030 | 0.518 | 3.439 |
| 6 | -0.361 | -0.302 | 2.343 |
| 6 | 0.178 | -1.598 | 2.910 |
| 6 | 1.019 | -1.375 | 4.160 |
| 8 | 0.460 | -0.511 | 5.058 |
| 8 | -1.421 | 1.735 | 2.835 |
| 8 | -1.242 | -0.655 | 1.305 |
| 8 | 1.043 | -2.255 | 1.967 |
| 26 | 3.109 | -1.837 | 1.996 |
| 8 | 2.783 | -0.217 | 0.777 |
| 8 | 2.292 | -0.879 | 3.648 |
| 6 | -0.600 | 1.491 | 5.742 |
| 8 | 0.457 | 1.851 | 6.610 |
| 17 | 5.148 | -1.264 | 2.486 |
| 8 | 3.193 | -3.634 | 2.972 |
| 8 | 3.228 | -2.935 | 0.264 |
| 1 | 0.085 | 2.308 | 7.372 |
| 1 | 0.834 | 1.330 | 4.166 |
| 1 | -1.328 | 0.841 | 6.245 |
| 1 | -1.123 | 2.380 | 5.368 |
| 1 | -2.284 | 2.003 | 3.168 |

| | | | |
|---|---|---|---|
| 1 | -1.900 | -0.027 | 3.829 |
| 1 | 0.475 | 0.298 | 1.952 |
| 1 | 1.211 | -2.308 | 4.695 |
| 1 | -0.646 | -2.277 | 3.152 |
| 1 | -1.563 | 0.161 | 0.899 |
| 1 | 0.556 | -2.492 | 1.162 |
| 1 | 2.198 | -0.170 | 0.007 |
| 1 | 3.495 | 0.426 | 0.650 |
| 1 | 4.006 | -4.021 | 3.326 |
| 1 | 2.500 | -4.309 | 2.961 |
| 1 | 3.624 | -2.553 | -0.532 |
| 1 | 3.507 | -3.860 | 0.312 |
| 1 | 2.899 | -0.697 | 4.384 |

$[Fe(H_2O)_3Cl]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 1.682 | 0.827 | 1.629 |
| 8 | 1.817 | 2.113 | 1.527 |
| 26 | 1.122 | 3.737 | 2.158 |
| 8 | 1.345 | 4.413 | 0.218 |
| 6 | 0.436 | 0.170 | 1.726 |
| 8 | -0.653 | 0.904 | 1.683 |
| 6 | 0.351 | -1.311 | 2.013 |
| 8 | 1.343 | -1.946 | 1.255 |
| 6 | 0.560 | -1.620 | 3.510 |
| 8 | 0.296 | -3.008 | 3.585 |
| 6 | -0.315 | -0.826 | 4.485 |
| 6 | -0.320 | -1.477 | 5.865 |
| 8 | -0.846 | -0.493 | 6.744 |
| 8 | 0.243 | 0.485 | 4.626 |
| 17 | 2.764 | 4.766 | 3.167 |
| 8 | 0.084 | 2.930 | 3.675 |
| 8 | -0.261 | 5.269 | 2.344 |
| 1 | -0.591 | -0.703 | 7.649 |
| 1 | -1.350 | -0.745 | 4.123 |
| 1 | 0.704 | -1.743 | 6.158 |
| 1 | -0.939 | -2.379 | 5.853 |
| 1 | 0.930 | -3.434 | 4.172 |
| 1 | 1.609 | -1.404 | 3.751 |
| 1 | -0.655 | -1.656 | 1.729 |
| 1 | 2.574 | 0.211 | 1.771 |
| 1 | 1.203 | 0.242 | 0.562 |
| 1 | 1.375 | -2.869 | 1.546 |
| 1 | -0.757 | 3.342 | 3.916 |
| 1 | 0.061 | 1.966 | 3.932 |
| 1 | -1.007 | 5.374 | 1.736 |
| 1 | 0.029 | 6.151 | 2.615 |
| 1 | 0.066 | 0.720 | 5.558 |
| 1 | 1.494 | 5.349 | 0.024 |
| 1 | 1.927 | 3.896 | -0.356 |
| 1 | -1.446 | 0.379 | 1.490 |

$[Fe(H_2O)_3Cl]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.765 | 0.636 | 1.897 |
| 6 | -2.185 | 0.381 | 1.764 |
| 6 | -2.583 | 0.883 | 0.366 |
| 6 | -1.307 | 1.572 | -0.131 |
| 6 | -0.208 | 0.835 | 0.650 |
| 6 | -2.449 | -1.089 | 2.001 |
| 1 | -2.041 | -1.384 | 2.972 |
| 8 | -3.690 | 1.743 | 0.480 |
| 8 | -1.161 | 1.512 | -1.537 |
| 6 | 1.137 | 1.523 | 0.820 |
| 8 | 1.909 | 1.184 | -0.343 |
| 26 | 1.746 | -0.734 | -1.133 |
| 8 | 0.083 | -0.431 | 0.023 |
| 8 | 0.541 | -0.137 | -2.650 |
| 8 | 0.975 | -2.599 | -1.527 |
| 8 | 2.608 | -1.692 | 0.480 |
| 8 | -1.819 | -1.830 | 0.948 |
| 1 | -3.528 | -1.274 | 1.986 |
| 1 | -4.113 | 1.826 | -0.383 |
| 1 | -1.117 | 2.403 | -1.904 |
| 1 | -0.161 | 0.494 | -2.321 |
| 1 | -1.321 | 2.612 | 0.208 |
| 1 | 1.026 | 2.606 | 0.881 |
| 1 | 2.773 | 1.621 | -0.338 |
| 1 | 1.626 | 1.141 | 1.720 |
| 1 | -0.597 | -1.127 | 0.332 |
| 1 | 0.537 | -2.733 | -2.380 |
| 1 | 1.491 | -3.391 | -1.325 |
| 1 | 3.563 | -1.683 | 0.631 |
| 1 | 2.164 | -1.843 | 1.326 |
| 1 | -2.813 | 0.044 | -0.302 |
| 1 | -2.697 | 0.970 | 2.530 |
| 1 | 0.940 | 0.222 | -3.454 |
| 1 | -1.732 | -2.759 | 1.193 |
| 17 | 3.646 | -0.586 | -2.214 |

$[Fe(H_2O)_3OH]^{2+}$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | 0.000 | 0.750 | 4.557 |
| 6 | -1.019 | 0.513 | 3.438 |
| 6 | -0.354 | -0.316 | 2.347 |
| 6 | 0.184 | -1.611 | 2.919 |
| 6 | 1.038 | -1.379 | 4.159 |
| 8 | 0.469 | -0.517 | 5.059 |
| 8 | -1.407 | 1.728 | 2.829 |
| 8 | -1.240 | -0.677 | 1.313 |
| 8 | 1.024 | -2.281 | 1.967 |
| 26 | 3.135 | -1.842 | 1.984 |
| 8 | 2.775 | -0.207 | 0.764 |
| 8 | 2.299 | -0.877 | 3.646 |
| 6 | -0.579 | 1.495 | 5.735 |
| 8 | 0.481 | 1.859 | 6.599 |
| 8 | 4.772 | -1.331 | 2.478 |
| 8 | 3.167 | -3.655 | 2.969 |
| 8 | 3.250 | -2.939 | 0.239 |
| 1 | 0.111 | 2.327 | 7.355 |
| 1 | 0.851 | 1.318 | 4.157 |
| 1 | -1.309 | 0.851 | 6.245 |
| 1 | -1.100 | 2.384 | 5.356 |
| 1 | -2.265 | 2.003 | 3.168 |
| 1 | -1.890 | -0.027 | 3.833 |
| 1 | 0.481 | 0.278 | 1.947 |
| 1 | 1.233 | -2.310 | 4.697 |
| 1 | -0.645 | -2.276 | 3.183 |
| 1 | -1.554 | 0.136 | 0.896 |
| 1 | 0.524 | -2.461 | 1.156 |
| 1 | 2.205 | -0.165 | -0.016 |
| 1 | 3.504 | 0.414 | 0.631 |
| 1 | 5.608 | -1.527 | 2.036 |
| 1 | 3.976 | -4.053 | 3.315 |
| 1 | 2.479 | -4.331 | 2.919 |
| 1 | 3.632 | -2.548 | -0.559 |
| 1 | 3.553 | -3.857 | 0.283 |
| 1 | 2.923 | -0.728 | 4.375 |

$[Fe(H_2O)_3OH]^{2+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 0.130 | -0.899 | 3.765 |
| 6 | 0.510 | -0.213 | 4.943 |
| 6 | 1.066 | -0.962 | 6.137 |
| 6 | 2.581 | -1.290 | 5.964 |
| 6 | 3.512 | -0.108 | 6.210 |
| 8 | 3.151 | 0.968 | 5.343 |
| 8 | -0.185 | -0.290 | 2.661 |
| 26 | 0.782 | 0.991 | 1.640 |
| 8 | 1.259 | 2.985 | 1.509 |
| 8 | 2.520 | 0.906 | 2.747 |
| 8 | 0.452 | 1.100 | 4.912 |
| 8 | 1.468 | 0.337 | 0.117 |
| 8 | -1.004 | 1.680 | 0.762 |
| 8 | 0.347 | -2.159 | 6.227 |
| 8 | 2.845 | -2.277 | 6.943 |
| 6 | 4.973 | -0.456 | 5.978 |
| 8 | 5.674 | 0.769 | 6.131 |
| 1 | 6.533 | 0.704 | 5.703 |
| 1 | 3.384 | 0.222 | 7.250 |
| 1 | 5.103 | -0.858 | 4.965 |
| 1 | 5.307 | -1.201 | 6.709 |
| 1 | 3.329 | -3.011 | 6.548 |
| 1 | 2.736 | -1.697 | 4.957 |
| 1 | 0.928 | -0.344 | 7.037 |
| 1 | 0.232 | -1.987 | 3.777 |
| 1 | -0.746 | -0.786 | 4.730 |
| 1 | 0.899 | -2.761 | 6.753 |
| 1 | 2.726 | 0.923 | 3.720 |
| 1 | 1.375 | -0.590 | -0.138 |
| 1 | -1.827 | 1.603 | 1.264 |
| 1 | -1.179 | 1.348 | -0.129 |
| 1 | 1.908 | 3.351 | 2.125 |
| 1 | 0.551 | 3.633 | 1.392 |
| 1 | 3.883 | 1.605 | 5.406 |
| 1 | 3.260 | 0.478 | 2.296 |
| 1 | 0.664 | 1.499 | 5.770 |

$[Fe(H_2O)_3OH]^{2+}$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | -0.763 | 0.625 | 1.896 |
| 6 | -2.188 | 0.398 | 1.777 |
| 6 | -2.585 | 0.885 | 0.375 |
| 6 | -1.307 | 1.560 | -0.131 |
| 6 | -0.210 | 0.809 | 0.642 |
| 6 | -2.481 | -1.063 | 2.040 |
| 1 | -2.075 | -1.348 | 3.016 |
| 8 | -3.689 | 1.751 | 0.481 |
| 8 | -1.173 | 1.496 | -1.538 |
| 6 | 1.139 | 1.492 | 0.809 |
| 8 | 1.905 | 1.169 | -0.360 |
| 26 | 1.780 | -0.759 | -1.161 |
| 8 | 3.375 | -0.615 | -1.960 |
| 8 | 0.066 | -0.454 | 0.018 |
| 8 | 0.547 | -0.149 | -2.677 |
| 8 | 0.987 | -2.633 | -1.561 |
| 8 | 2.578 | -1.720 | 0.504 |
| 8 | -1.873 | -1.833 | 0.999 |
| 1 | -3.565 | -1.223 | 2.038 |
| 1 | -4.109 | 1.830 | -0.384 |
| 1 | -1.129 | 2.386 | -1.906 |
| 1 | -0.156 | 0.468 | -2.333 |
| 1 | -1.307 | 2.601 | 0.205 |
| 1 | 1.029 | 2.574 | 0.891 |
| 1 | 2.768 | 1.607 | -0.352 |
| 1 | 1.630 | 1.095 | 1.702 |
| 1 | -0.607 | -1.136 | 0.333 |
| 1 | 0.579 | -2.770 | -2.427 |
| 1 | 1.504 | -3.421 | -1.345 |
| 1 | 3.661 | -1.043 | -2.776 |
| 1 | 3.532 | -1.699 | 0.658 |
| 1 | 2.133 | -1.797 | 1.358 |

| | | | |
|---|---|---|---|
| 1 | -2.821 | 0.039 | -0.282 |
| 1 | -2.682 | 1.009 | 2.537 |
| 1 | 0.953 | 0.251 | -3.456 |
| 1 | -1.810 | -2.759 | 1.259 |

$[Fe(H_2O)_2Cl_2]^+$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -1.041 | 0.435 | 3.408 |
| 6 | -0.379 | -0.300 | 2.261 |
| 6 | 0.910 | 0.372 | 1.805 |
| 8 | 1.730 | 0.727 | 2.849 |
| 6 | 1.138 | 1.503 | 3.906 |
| 6 | -0.033 | 0.722 | 4.512 |
| 8 | -1.242 | -0.345 | 1.117 |
| 26 | -1.120 | 1.191 | -0.376 |
| 8 | 0.094 | -0.291 | -1.231 |
| 8 | 0.484 | 1.515 | 1.034 |
| 6 | 2.235 | 1.796 | 4.900 |
| 8 | 3.147 | 2.700 | 4.305 |
| 8 | -0.716 | 1.486 | 5.487 |
| 8 | -2.108 | -0.384 | 3.833 |
| 8 | -2.097 | 2.525 | 0.909 |
| 1 | 3.844 | 2.893 | 4.942 |
| 1 | 0.767 | 2.452 | 3.496 |
| 1 | 2.730 | 0.855 | 5.180 |
| 1 | 1.778 | 2.232 | 5.797 |
| 1 | -0.456 | 1.198 | 6.368 |
| 1 | 0.330 | -0.225 | 4.935 |
| 1 | -1.426 | 1.399 | 3.046 |
| 1 | 1.496 | -0.285 | 1.157 |
| 1 | -0.150 | -1.327 | 2.565 |
| 1 | -2.604 | 0.100 | 4.505 |
| 1 | -2.120 | -0.661 | 1.382 |
| 1 | -1.650 | 3.357 | 1.120 |
| 1 | 0.412 | -0.127 | -2.129 |
| 1 | 1.256 | 1.948 | 0.638 |
| 1 | -3.009 | 2.743 | 0.668 |
| 1 | -0.232 | -1.201 | -1.199 |
| 17 | -0.247 | 2.721 | -1.728 |
| 17 | -3.053 | 0.534 | -1.236 |

$[Fe(H_2O)_2Cl_2]^+$-TS2

| | | | |
|---|---|---|---|
| 6 | 1.770 | 1.071 | 2.352 |
| 8 | 2.104 | 2.296 | 2.632 |
| 26 | 1.177 | 3.945 | 2.291 |
| 17 | -0.789 | 4.906 | 1.852 |
| 6 | 0.429 | 0.684 | 2.139 |
| 8 | -0.452 | 1.660 | 2.178 |
| 6 | 0.018 | -0.756 | 1.916 |
| 8 | 0.948 | -1.312 | 1.023 |
| 6 | -0.007 | -1.594 | 3.212 |
| 8 | -0.395 | -2.879 | 2.762 |
| 6 | -0.952 | -1.056 | 4.279 |
| 6 | -1.083 | -1.994 | 5.466 |
| 8 | -1.867 | -1.291 | 6.419 |
| 8 | -0.406 | 0.182 | 4.697 |
| 8 | 0.732 | 3.951 | 4.334 |
| 17 | 2.752 | 5.477 | 2.237 |
| 8 | 1.254 | 3.280 | 0.269 |
| 1 | -1.791 | -1.725 | 7.275 |
| 1 | -1.953 | -0.906 | 3.843 |
| 1 | -0.087 | -2.220 | 5.872 |
| 1 | -1.570 | -2.928 | 5.162 |
| 1 | 0.097 | -3.556 | 3.239 |
| 1 | 1.013 | -1.613 | 3.620 |
| 1 | -0.997 | -0.757 | 1.487 |
| 1 | 2.519 | 0.282 | 2.442 |
| 1 | 1.386 | 0.891 | 1.120 |
| 1 | 0.798 | -2.270 | 1.037 |
| 1 | 2.110 | 3.338 | -0.179 |
| 1 | 0.598 | 3.675 | -0.321 |
| 1 | -0.875 | 0.432 | 5.505 |
| 1 | -0.159 | 4.223 | 4.593 |
| 1 | 0.956 | 3.156 | 4.836 |
| 1 | -1.302 | 1.430 | 1.775 |

$[Fe(H_2O)_2Cl_2]^+$-fructofuranose complex

| | | | |
|---|---|---|---|
| 8 | 1.306 | 1.131 | -2.288 |
| 6 | -0.046 | 0.769 | -1.960 |
| 6 | -0.933 | 1.610 | -2.880 |
| 6 | 0.017 | 2.075 | -4.011 |
| 6 | 1.382 | 1.451 | -3.629 |
| 6 | -0.276 | -0.725 | -2.131 |
| 8 | 0.807 | -1.412 | -1.507 |
| 8 | -1.453 | 2.685 | -2.130 |
| 8 | -0.402 | 1.600 | -5.273 |
| 6 | 2.617 | 2.288 | -3.881 |
| 8 | 3.716 | 1.383 | -3.731 |
| 26 | 3.485 | -0.610 | -4.547 |
| 8 | 3.615 | 0.451 | -6.401 |
| 8 | 1.543 | 0.242 | -4.399 |
| 17 | 2.661 | -2.389 | -5.607 |
| 8 | 3.168 | -1.281 | -2.652 |
| 17 | 5.699 | -0.856 | -4.407 |
| 1 | 0.570 | -2.342 | -1.399 |
| 1 | -0.334 | -1.004 | -3.189 |
| 1 | -1.223 | -0.988 | -1.647 |
| 1 | -2.122 | 3.140 | -2.656 |
| 1 | -0.281 | 2.281 | -5.945 |
| 1 | 0.087 | 3.166 | -3.990 |
| 1 | 2.599 | 2.693 | -4.898 |
| 1 | 4.564 | 1.835 | -3.841 |
| 1 | 2.692 | 3.095 | -3.149 |
| 1 | 0.937 | 0.312 | -5.170 |
| 1 | 3.789 | -0.958 | -1.987 |
| 1 | 2.252 | -1.282 | -2.240 |
| 1 | -1.740 | 1.013 | -3.323 |
| 1 | -0.186 | 1.053 | -0.915 |
| 1 | 3.281 | -0.055 | -7.155 |
| 1 | 4.508 | 0.736 | -6.641 |

$[Fe_2(H_2O)_7OH]^{5+}$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.139 | 0.974 | 1.423 |
| 8 | 2.281 | 2.262 | 1.467 |
| 26 | 0.425 | 3.297 | 2.128 |
| 8 | -0.068 | 3.724 | 0.183 |
| 6 | 0.817 | 0.525 | 1.665 |
| 8 | -0.072 | 1.451 | 1.949 |
| 6 | 0.475 | -0.925 | 1.913 |
| 8 | 1.384 | -1.684 | 1.164 |
| 6 | 0.578 | -1.295 | 3.407 |
| 8 | 0.300 | -2.685 | 3.407 |
| 6 | -0.374 | -0.510 | 4.326 |
| 6 | -0.931 | -1.366 | 5.455 |
| 8 | -1.552 | -0.446 | 6.342 |
| 8 | 0.359 | 0.565 | 4.938 |
| 26 | 3.610 | 3.723 | 1.687 |
| 8 | 3.774 | 3.182 | 3.658 |
| 8 | 3.812 | 3.886 | -0.344 |
| 8 | 1.927 | 4.601 | 1.976 |
| 8 | 4.830 | 5.316 | 1.892 |
| 8 | 5.268 | 2.552 | 1.526 |
| 8 | -1.500 | 3.538 | 2.758 |
| 8 | 1.043 | 2.850 | 4.062 |
| 1 | -1.652 | -0.853 | 7.210 |
| 1 | -1.212 | -0.082 | 3.760 |
| 1 | -0.120 | -1.900 | 5.965 |
| 1 | -1.646 | -2.092 | 5.059 |
| 1 | 0.885 | -3.135 | 4.027 |
| 1 | 1.605 | -1.108 | 3.746 |
| 1 | -0.562 | -1.088 | 1.585 |
| 1 | 2.969 | 0.301 | 1.218 |
| 1 | 1.201 | 0.552 | 0.433 |
| 1 | 1.304 | -2.597 | 1.476 |
| 1 | 0.732 | 1.922 | 4.378 |
| 1 | 0.760 | 3.489 | 4.735 |
| 1 | 1.804 | 5.509 | 2.288 |
| 1 | 0.086 | 4.603 | -0.192 |
| 1 | -0.853 | 3.350 | -0.242 |
| 1 | -2.112 | 2.797 | 2.638 |
| 1 | -1.990 | 4.363 | 2.630 |
| 1 | -0.110 | 0.728 | 5.780 |
| 1 | 5.574 | 1.957 | 2.225 |
| 1 | 3.164 | 3.497 | -0.949 |
| 1 | 2.892 | 3.017 | 4.060 |
| 1 | 5.795 | 5.247 | 1.922 |
| 1 | 4.284 | 3.735 | 4.268 |
| 1 | 4.579 | 6.240 | 2.034 |
| 1 | 4.132 | 4.710 | -0.740 |
| 1 | 5.637 | 2.265 | 0.678 |

$[Fe(H_2O)Cl_3]$-glucopyranose complex

| | | | |
|---|---|---|---|
| 6 | -0.046 | 0.773 | 4.503 |
| 6 | -1.029 | 0.506 | 3.373 |
| 6 | -0.356 | -0.270 | 2.261 |
| 6 | 0.943 | 0.387 | 1.813 |
| 8 | 1.761 | 0.695 | 2.885 |
| 6 | 1.178 | 1.494 | 3.926 |
| 8 | -2.137 | -0.270 | 3.778 |
| 8 | -1.207 | -0.353 | 1.110 |
| 26 | -1.095 | 1.120 | -0.415 |
| 17 | -2.828 | 0.205 | -1.507 |
| 8 | 0.552 | 1.545 | 1.072 |
| 6 | 2.257 | 1.731 | 4.954 |
| 8 | 3.230 | 2.596 | 4.397 |
| 8 | -0.726 | 1.583 | 5.444 |
| 17 | 0.572 | -0.014 | -1.564 |
| 17 | -2.309 | 2.722 | 0.711 |
| 8 | -0.404 | 2.759 | -1.533 |
| 1 | 3.919 | 2.744 | 5.053 |
| 1 | 0.862 | 2.461 | 3.511 |
| 1 | 2.699 | 0.767 | 5.241 |
| 1 | 1.795 | 2.182 | 5.841 |
| 1 | -0.496 | 1.308 | 6.337 |
| 1 | 0.262 | -0.180 | 4.955 |
| 1 | -1.367 | 1.475 | 2.980 |
| 1 | 1.520 | -0.278 | 1.166 |
| 1 | -0.136 | -1.289 | 2.599 |
| 1 | -2.650 | 0.252 | 4.408 |
| 1 | -2.097 | -0.620 | 1.390 |
| 1 | 1.326 | 1.895 | 0.605 |
| 1 | -0.990 | 3.525 | -1.600 |
| 1 | -0.030 | 2.574 | -2.406 |

$[Fe(H_2O)Cl_3]$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.418 | 0.985 | 1.309 |
| 8 | 1.451 | 0.626 | 2.099 |
| 26 | 0.880 | -1.249 | 2.235 |
| 17 | 0.990 | -1.102 | 4.545 |

| | | | |
|---|---|---|---|
| 6 | 3.392 | 0.033 | 0.934 |
| 8 | 3.170 | -1.174 | 1.406 |
| 6 | 4.627 | 0.321 | 0.117 |
| 8 | 4.669 | 1.697 | -0.120 |
| 6 | 5.907 | -0.167 | 0.876 |
| 8 | 6.971 | 0.667 | 0.466 |
| 6 | 6.280 | -1.600 | 0.492 |
| 6 | 7.293 | -2.217 | 1.439 |
| 8 | 7.403 | -3.575 | 1.039 |
| 8 | 5.105 | -2.417 | 0.478 |
| 17 | 1.232 | -3.494 | 2.169 |
| 17 | 0.317 | -1.106 | -0.071 |
| 8 | -1.179 | -1.036 | 2.500 |
| 1 | 7.812 | -4.085 | 1.746 |
| 1 | 6.692 | -1.576 | -0.525 |
| 1 | 6.930 | -2.144 | 2.472 |
| 1 | 8.251 | -1.691 | 1.355 |
| 1 | 7.343 | 1.123 | 1.229 |
| 1 | 5.748 | -0.082 | 1.958 |
| 1 | 4.556 | -0.234 | -0.832 |
| 1 | 2.591 | 2.036 | 1.077 |
| 1 | 2.286 | 0.461 | 0.119 |
| 1 | 5.608 | 1.913 | -0.248 |
| 1 | -1.538 | -1.377 | 3.330 |
| 1 | 5.390 | -3.335 | 0.624 |
| 1 | 3.860 | -1.848 | 1.060 |
| 1 | -1.728 | -1.355 | 1.771 |

$[Fe(H_2O)Cl_3]$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | 1.477 | 1.328 | -3.561 |
| 8 | 1.269 | 0.784 | -2.308 |
| 6 | -0.131 | 0.774 | -1.961 |
| 6 | -0.873 | 1.283 | -3.191 |
| 6 | 0.193 | 2.094 | -3.924 |
| 6 | -0.563 | -0.603 | -1.521 |
| 8 | 0.054 | -0.893 | -0.280 |
| 8 | -1.999 | 2.023 | -2.792 |
| 8 | -0.047 | 2.085 | -5.313 |
| 6 | 2.763 | 2.131 | -3.589 |
| 8 | 3.833 | 1.185 | -3.564 |
| 26 | 3.536 | -0.496 | -4.986 |
| 8 | 5.636 | -0.636 | -5.050 |
| 8 | 1.617 | 0.261 | -4.534 |
| 17 | 3.887 | 1.142 | -6.624 |
| 17 | 2.716 | -2.022 | -6.425 |
| 17 | 3.708 | -1.896 | -3.179 |
| 1 | -0.190 | -1.787 | -0.017 |
| 1 | -0.279 | -1.334 | -2.289 |
| 1 | -1.658 | -0.600 | -1.429 |
| 1 | -2.584 | 2.133 | -3.550 |
| 1 | 0.281 | 2.896 | -5.719 |
| 1 | 0.230 | 3.111 | -3.518 |
| 1 | 2.812 | 2.724 | -4.508 |
| 1 | 4.667 | 1.638 | -3.753 |
| 1 | 2.815 | 2.783 | -2.713 |
| 1 | 1.131 | 0.556 | -5.334 |
| 1 | -1.168 | 0.444 | -3.838 |
| 1 | -0.273 | 1.482 | -1.134 |
| 1 | 6.030 | -1.442 | -4.691 |
| 1 | 6.059 | -0.435 | -5.897 |

$[Fe(OH)Cl_3]^-$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.484 | 0.195 | 1.750 |
| 8 | 1.601 | -0.265 | 2.582 |
| 26 | -0.253 | -0.803 | 2.294 |
| 17 | -0.681 | -0.347 | 4.604 |
| 6 | 3.491 | -0.606 | 1.183 |
| 8 | 3.544 | -1.888 | 1.498 |
| 6 | 4.565 | -0.035 | 0.274 |
| 8 | 4.321 | 1.326 | 0.068 |
| 6 | 5.985 | -0.269 | 0.899 |
| 8 | 6.789 | 0.849 | 0.570 |
| 6 | 6.657 | -1.508 | 0.310 |
| 6 | 7.875 | -1.944 | 1.101 |
| 8 | 8.291 | -3.170 | 0.518 |
| 8 | 5.712 | -2.575 | 0.277 |
| 17 | -0.522 | -3.075 | 2.479 |
| 17 | 0.375 | -0.958 | -0.125 |
| 8 | -1.784 | 0.094 | 1.775 |
| 1 | 8.889 | -3.623 | 1.122 |
| 1 | 6.955 | -1.268 | -0.721 |
| 1 | 7.599 | -2.089 | 2.154 |
| 1 | 8.657 | -1.179 | 1.036 |
| 1 | 7.091 | 1.282 | 1.376 |
| 1 | 5.895 | -0.363 | 1.988 |
| 1 | 4.516 | -0.575 | -0.684 |
| 1 | 2.531 | 1.260 | 1.513 |
| 1 | 2.272 | -0.308 | 0.524 |
| 1 | 5.199 | 1.743 | 0.018 |
| 1 | -2.300 | 0.366 | 2.544 |
| 1 | 6.213 | -3.405 | 0.261 |
| 1 | 4.300 | -2.327 | 1.020 |

$[Fe(H_2O)_2OHCl]^+$-glucopyranose complex

| | | | |
|---|---|---|---|
| 8 | -0.002 | 0.770 | 4.547 |
| 6 | -0.948 | 0.544 | 3.489 |
| 6 | -0.299 | -0.316 | 2.399 |
| 6 | 0.944 | 0.402 | 1.895 |
| 6 | 1.888 | 0.696 | 3.043 |
| 6 | 1.180 | 1.389 | 4.201 |
| 6 | -2.157 | -0.110 | 4.116 |
| 8 | -2.809 | 0.842 | 4.936 |
| 8 | -1.155 | -0.472 | 1.282 |
| 8 | 1.682 | -0.364 | 0.967 |
| 8 | 2.945 | 1.566 | 2.623 |
| 26 | 2.687 | 3.724 | 2.833 |
| 17 | 4.502 | 4.099 | 1.573 |
| 8 | 0.981 | 2.743 | 3.764 |
| 8 | 1.450 | 3.664 | 1.109 |
| 8 | 2.032 | 5.258 | 3.538 |
| 8 | 3.721 | 3.251 | 4.621 |
| 1 | -3.579 | 0.424 | 5.336 |
| 1 | -1.249 | 1.508 | 3.057 |
| 1 | -1.832 | -0.983 | 4.700 |
| 1 | -2.818 | -0.453 | 3.311 |
| 1 | -1.575 | -1.338 | 1.312 |
| 1 | -0.015 | -1.292 | 2.816 |
| 1 | 0.627 | 1.349 | 1.437 |
| 1 | 1.801 | 1.395 | 5.100 |
| 1 | 2.324 | -0.239 | 3.409 |
| 1 | 1.130 | -0.495 | 0.186 |
| 1 | 3.337 | 1.223 | 1.806 |
| 1 | 1.917 | 3.857 | 0.284 |
| 1 | 0.690 | 4.263 | 1.143 |
| 1 | 2.395 | 6.115 | 3.285 |
| 1 | 3.965 | 4.018 | 5.158 |
| 1 | 4.510 | 2.699 | 4.536 |
| 1 | 0.627 | 3.279 | 4.489 |

$[Fe(H_2O)_2OHCl]^+$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.190 | 1.028 | 1.172 |
| 8 | 2.285 | 2.305 | 0.964 |
| 26 | 1.109 | 3.742 | 1.568 |
| 8 | 1.962 | 3.502 | 3.508 |
| 6 | 1.052 | 0.467 | 1.803 |
| 8 | 0.099 | 1.317 | 2.113 |
| 6 | 0.937 | -0.987 | 2.206 |
| 8 | 2.104 | -1.642 | 1.810 |
| 6 | 0.718 | -1.093 | 3.755 |
| 8 | 1.311 | -2.304 | 4.175 |
| 6 | -0.769 | -1.162 | 4.106 |
| 6 | -1.035 | -0.932 | 5.582 |
| 8 | -2.448 | -0.859 | 5.703 |
| 8 | -1.479 | -0.179 | 3.348 |
| 17 | -0.782 | 4.428 | 2.607 |
| 8 | -0.058 | 3.452 | -0.189 |
| 8 | 2.069 | 5.168 | 1.013 |
| 1 | -2.677 | -0.456 | 6.547 |
| 1 | -1.136 | -2.155 | 3.814 |
| 1 | -0.569 | 0.009 | 5.902 |
| 1 | -0.620 | -1.758 | 6.170 |
| 1 | 1.998 | -2.124 | 4.827 |
| 1 | 1.193 | -0.240 | 4.253 |
| 1 | 0.060 | -1.418 | 1.700 |
| 1 | 3.047 | 0.378 | 0.997 |
| 1 | 1.301 | 0.413 | 0.426 |
| 1 | 2.235 | -2.360 | 2.453 |
| 1 | 1.738 | 6.061 | 1.165 |
| 1 | -2.292 | 0.031 | 3.838 |
| 1 | -0.670 | 0.844 | 2.584 |
| 1 | -0.955 | 3.114 | -0.071 |
| 1 | 0.334 | 2.977 | -0.932 |
| 1 | 1.356 | 3.297 | 4.231 |
| 1 | 2.753 | 2.959 | 3.626 |

$[Fe(H_2O)_2OHCl]^+$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.727 | 0.596 | 1.858 |
| 8 | -2.089 | 0.351 | 1.767 |
| 6 | -2.590 | 0.823 | 0.495 |
| 6 | -1.517 | 1.769 | -0.066 |
| 6 | -0.552 | 1.927 | 1.111 |
| 6 | -2.902 | -0.366 | -0.389 |
| 8 | -1.675 | -1.041 | -0.674 |
| 8 | -2.126 | 2.969 | -0.481 |
| 8 | 0.778 | 2.187 | 0.705 |
| 6 | -0.328 | 0.552 | 3.325 |
| 8 | 1.073 | 0.285 | 3.356 |
| 26 | 1.821 | -1.272 | 1.978 |
| 8 | 0.580 | -2.625 | 3.062 |
| 8 | 0.020 | -0.443 | 1.212 |
| 8 | 3.188 | -1.480 | 3.160 |
| 8 | 2.689 | 0.340 | 0.988 |
| 17 | 2.031 | -2.715 | 0.266 |
| 1 | -3.597 | -1.033 | 0.128 |
| 1 | -3.362 | -0.015 | -1.320 |
| 1 | -1.522 | 3.438 | -1.068 |
| 1 | 1.051 | 3.058 | 1.015 |
| 1 | 2.029 | 1.065 | 0.847 |
| 1 | -0.920 | 2.730 | 1.758 |
| 1 | -0.545 | 1.503 | 3.816 |
| 1 | 1.391 | 0.211 | 4.265 |
| 1 | -0.886 | -0.252 | 3.815 |
| 1 | -0.522 | -0.821 | 0.459 |
| 1 | 3.824 | -2.193 | 3.033 |
| 1 | 0.699 | -2.745 | 4.012 |
| 1 | -0.348 | -2.787 | 2.852 |
| 1 | -0.980 | 1.302 | -0.900 |

| | | | |
|---|---|---|---|
| 1 | -3.510 | 1.381 | 0.688 |
| 1 | 3.437 | 0.712 | 1.471 |
| 1 | -1.851 | -1.933 | -0.994 |

$[Fe(H_2O)_2OH_2]^+$-glucopyranose complex

| | | | |
|---|---|---|---|
| 8 | 0.023 | 0.778 | 4.533 |
| 6 | -0.937 | 0.547 | 3.490 |
| 6 | -0.302 | -0.327 | 2.402 |
| 6 | 0.937 | 0.383 | 1.876 |
| 6 | 1.894 | 0.695 | 3.008 |
| 6 | 1.196 | 1.410 | 4.160 |
| 6 | -2.142 | -0.094 | 4.135 |
| 8 | -2.782 | 0.870 | 4.951 |
| 8 | -1.169 | -0.497 | 1.296 |
| 8 | 1.663 | -0.398 | 0.949 |
| 8 | 2.951 | 1.548 | 2.563 |
| 26 | 2.738 | 3.731 | 2.739 |
| 8 | 4.188 | 3.927 | 1.648 |
| 8 | 0.978 | 2.746 | 3.704 |
| 8 | 1.424 | 3.631 | 1.047 |
| 8 | 2.067 | 5.255 | 3.501 |
| 8 | 3.720 | 3.234 | 4.590 |
| 1 | -3.549 | 0.459 | 5.365 |
| 1 | -1.238 | 1.507 | 3.050 |
| 1 | -1.816 | -0.962 | 4.726 |
| 1 | -2.814 | -0.443 | 3.341 |
| 1 | -1.602 | -1.355 | 1.352 |
| 1 | -0.013 | -1.298 | 2.828 |
| 1 | 0.616 | 1.323 | 1.406 |
| 1 | 1.827 | 1.432 | 5.052 |
| 1 | 2.325 | -0.238 | 3.389 |
| 1 | 1.099 | -0.543 | 0.179 |
| 1 | 3.314 | 1.199 | 1.735 |
| 1 | 1.851 | 3.978 | 0.253 |
| 1 | 0.591 | 4.112 | 1.148 |
| 1 | 2.416 | 6.114 | 3.237 |
| 1 | 3.886 | 4.018 | 5.129 |
| 1 | 4.559 | 2.760 | 4.515 |
| 1 | 4.633 | 4.779 | 1.577 |
| 1 | 0.667 | 3.302 | 4.434 |

$[Fe(H_2O)_2OH_2]^+$-TS2 complex

| | | | |
|---|---|---|---|
| 6 | 0.129 | -0.641 | 3.812 |
| 8 | 0.575 | -0.003 | 4.848 |
| 26 | 1.473 | -0.662 | 6.441 |
| 8 | 0.083 | 0.682 | 7.428 |
| 6 | -0.377 | -1.964 | 3.870 |
| 8 | -0.439 | -2.547 | 5.044 |
| 6 | -0.754 | -2.749 | 2.628 |
| 8 | -0.621 | -1.924 | 1.510 |
| 6 | 0.169 | -4.014 | 2.519 |
| 8 | 0.387 | -4.259 | 1.144 |
| 6 | -0.512 | -5.248 | 3.112 |
| 6 | 0.450 | -6.399 | 3.334 |
| 8 | -0.301 | -7.394 | 4.013 |
| 8 | -1.113 | -4.894 | 4.358 |
| 8 | 1.262 | -1.977 | 7.697 |
| 8 | 2.491 | -2.082 | 5.104 |
| 8 | 3.003 | 0.268 | 6.805 |
| 1 | 0.300 | -8.037 | 4.405 |
| 1 | -1.304 | -5.559 | 2.418 |
| 1 | 1.296 | -6.064 | 3.949 |
| 1 | 0.826 | -6.763 | 2.371 |
| 1 | 1.331 | -4.240 | 0.953 |
| 1 | 1.121 | -3.816 | 3.026 |
| 1 | -1.797 | -3.082 | 2.736 |
| 1 | 0.249 | -0.214 | 2.814 |
| 1 | -1.172 | -0.814 | 3.794 |
| 1 | -0.301 | -2.500 | 0.794 |
| 1 | 2.609 | -2.913 | 5.584 |
| 1 | 3.161 | 1.106 | 6.356 |
| 1 | -0.313 | 0.307 | 8.225 |
| 1 | -0.646 | 0.946 | 6.852 |
| 1 | 0.481 | -2.540 | 7.649 |
| 1 | -1.199 | -5.708 | 4.881 |
| 1 | 3.379 | -1.772 | 4.881 |
| 1 | -0.777 | -3.492 | 4.947 |

$[Fe(H_2O)_2OH_2]^+$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.551 | 1.925 | 1.117 |
| 6 | -0.717 | 0.568 | 1.820 |
| 8 | -2.083 | 0.330 | 1.738 |
| 6 | -2.600 | 0.849 | 0.491 |
| 6 | -1.529 | 1.807 | -0.052 |
| 6 | -0.300 | 0.478 | 3.279 |
| 8 | 1.101 | 0.223 | 3.283 |
| 26 | 1.851 | -1.327 | 1.825 |
| 8 | 2.036 | -2.454 | 0.392 |
| 8 | 0.018 | -0.447 | 1.132 |
| 6 | -2.935 | -0.304 | -0.431 |
| 8 | -1.719 | -0.977 | -0.763 |
| 8 | -2.136 | 3.022 | -0.426 |
| 8 | 0.772 | 2.204 | 0.701 |
| 8 | 0.611 | -2.749 | 2.842 |
| 8 | 3.190 | -1.523 | 3.076 |
| 8 | 2.702 | 0.338 | 0.855 |
| 1 | -3.627 | -0.985 | 0.074 |
| 1 | -3.410 | 0.085 | -1.339 |
| 1 | -1.529 | 3.511 | -0.993 |
| 1 | 1.063 | 3.040 | 1.081 |
| 1 | 2.032 | 1.060 | 0.763 |
| 1 | -0.913 | 2.705 | 1.795 |
| 1 | -0.525 | 1.410 | 3.803 |
| 1 | 1.425 | 0.086 | 4.183 |
| 1 | -0.849 | -0.347 | 3.748 |
| 1 | -0.529 | -0.797 | 0.375 |
| 1 | 2.421 | -2.087 | -0.412 |
| 1 | 3.866 | -2.186 | 2.896 |
| 1 | 0.752 | -2.888 | 3.786 |
| 1 | -0.335 | -2.835 | 2.670 |
| 1 | -1.003 | 1.362 | -0.906 |
| 1 | -3.513 | 1.407 | 0.717 |
| 1 | 3.452 | 0.700 | 1.342 |
| 1 | -1.909 | -1.854 | -1.114 |

$[Fe(H_2O)OHCl_2]$-glucopyranose complex

| | | | |
|---|---|---|---|
| 8 | 1.798 | 0.751 | 2.851 |
| 6 | 1.184 | 1.523 | 3.893 |
| 6 | -0.029 | 0.765 | 4.445 |
| 6 | -0.993 | 0.493 | 3.300 |
| 6 | -0.294 | -0.249 | 2.179 |
| 6 | 0.998 | 0.443 | 1.763 |
| 6 | 2.244 | 1.773 | 4.939 |
| 8 | 3.204 | 2.666 | 4.403 |
| 8 | -0.740 | 1.542 | 5.392 |
| 8 | -2.088 | -0.311 | 3.687 |
| 8 | -1.119 | -0.316 | 1.014 |
| 26 | -1.046 | 1.325 | -0.451 |
| 17 | -2.404 | 2.761 | 0.681 |
| 8 | 0.591 | 1.603 | 1.038 |
| 8 | -0.135 | 2.465 | -1.574 |
| 17 | -2.617 | 0.179 | -1.660 |
| 8 | 0.509 | -0.064 | -1.250 |
| 1 | 3.879 | 2.827 | 5.072 |
| 1 | 0.850 | 2.487 | 3.486 |
| 1 | 2.705 | 0.816 | 5.222 |
| 1 | 1.760 | 2.205 | 5.824 |
| 1 | -0.508 | 1.262 | 6.283 |
| 1 | 0.297 | -0.188 | 4.884 |
| 1 | -1.351 | 1.461 | 2.920 |
| 1 | 1.597 | -0.199 | 1.113 |
| 1 | -0.056 | -1.268 | 2.505 |
| 1 | -2.601 | 0.183 | 4.339 |
| 1 | -2.002 | -0.627 | 1.263 |
| 1 | 1.346 | 1.984 | 0.566 |
| 1 | 0.846 | 0.406 | -2.026 |
| 1 | 0.132 | -0.892 | -1.575 |
| 1 | -0.446 | 3.377 | -1.607 |

$[Fe(H_2O)OHCl_2]$-TS2

| | | | |
|---|---|---|---|
| 6 | 2.716 | 1.271 | 1.464 |
| 6 | 2.717 | 2.650 | 1.147 |
| 6 | 1.498 | 3.532 | 1.368 |
| 6 | 1.857 | 4.678 | 2.379 |
| 6 | 2.241 | 5.967 | 1.651 |
| 8 | 3.110 | 5.650 | 0.564 |
| 8 | 3.757 | 0.508 | 1.396 |
| 26 | 5.048 | 0.117 | -0.036 |
| 8 | 5.223 | -1.687 | -0.260 |
| 8 | 6.314 | -0.016 | 1.780 |
| 17 | 6.826 | 1.264 | -0.925 |
| 17 | 3.461 | 0.608 | -1.657 |
| 8 | 3.839 | 3.210 | 0.749 |
| 8 | 0.442 | 2.751 | 1.841 |
| 8 | 0.698 | 4.949 | 3.143 |
| 6 | 2.931 | 6.968 | 2.560 |
| 8 | 3.350 | 8.027 | 1.712 |
| 1 | 4.018 | 8.554 | 2.164 |
| 1 | 1.320 | 6.409 | 1.247 |
| 1 | 3.795 | 6.493 | 3.043 |
| 1 | 2.235 | 7.318 | 3.330 |
| 1 | 0.882 | 4.808 | 4.078 |
| 1 | 2.673 | 4.347 | 3.032 |
| 1 | 1.231 | 3.991 | 0.404 |
| 1 | 1.786 | 0.884 | 1.886 |
| 1 | 2.279 | 1.677 | 0.263 |
| 1 | -0.045 | 3.319 | 2.463 |
| 1 | 4.752 | -2.067 | -1.010 |
| 1 | 3.626 | 6.449 | 0.366 |
| 1 | 3.690 | 4.180 | 0.547 |
| 1 | 7.125 | 0.500 | 1.678 |
| 1 | 5.829 | 0.370 | 2.521 |

$[Fe(H_2O)OHCl_2]$-fructofuranose complex

| | | | |
|---|---|---|---|
| 6 | -0.783 | 1.268 | -3.143 |
| 6 | 0.263 | 2.114 | -3.872 |
| 6 | 1.546 | 1.305 | -3.643 |
| 8 | 1.400 | 0.694 | -2.396 |
| 6 | 0.007 | 0.622 | -2.008 |
| 8 | -0.050 | 2.217 | -5.241 |
| 6 | 2.851 | 2.073 | -3.683 |
| 8 | 3.882 | 1.090 | -3.618 |
| 26 | 3.576 | -0.731 | -4.933 |
| 17 | 2.529 | -2.426 | -6.051 |
| 8 | 1.610 | 0.272 | -4.634 |
| 6 | -0.383 | -0.810 | -1.734 |
| 8 | 0.401 | -1.278 | -0.653 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 8 | -1.855 | 2.002 | -2.609 | 1 | 2.338 | -0.542 | -0.772 |
| 8 | 2.994 | -1.496 | -2.993 | 1 | 3.175 | 4.034 | -1.063 |
| 8 | 5.247 | -1.322 | -4.457 | | | | |
| 17 | 4.048 | 0.649 | -6.715 | | | | |
| 1 | 0.191 | -2.205 | -0.497 | | | | |
| 1 | -0.216 | -1.414 | -2.637 | | | | |
| 1 | -1.455 | -0.832 | -1.495 | | | | |
| 1 | -2.485 | 2.192 | -3.314 | | | | |
| 1 | 0.242 | 3.067 | -5.590 | | | | |
| 1 | 0.343 | 3.095 | -3.390 | | | | |
| 1 | 2.920 | 2.635 | -4.621 | | | | |
| 1 | 4.734 | 1.490 | -3.833 | | | | |
| 1 | 2.917 | 2.753 | -2.830 | | | | |
| 1 | 1.188 | 0.617 | -5.444 | | | | |
| 1 | -1.146 | 0.503 | -3.844 | | | | |
| 1 | -0.103 | 1.219 | -1.096 | | | | |
| 1 | 3.812 | -1.622 | -2.494 | | | | |
| 1 | 2.440 | -0.869 | -2.486 | | | | |
| 1 | 5.948 | -1.227 | -5.113 | | | | |
| without catalyst – TS2 trans | | | | | | | |
| 6 | -1.089 | 0.762 | 2.477 | | | | |
| 8 | -0.429 | 1.615 | 1.800 | | | | |
| 6 | -0.729 | 0.125 | 3.742 | | | | |
| 8 | -1.563 | -0.465 | 4.505 | | | | |
| 6 | 0.701 | 0.385 | 4.228 | | | | |
| 8 | 0.611 | 1.495 | 5.114 | | | | |
| 6 | 1.314 | -0.812 | 4.974 | | | | |
| 8 | 2.337 | -0.288 | 5.828 | | | | |
| 6 | 1.961 | -1.839 | 4.047 | | | | |
| 6 | 2.573 | -3.000 | 4.814 | | | | |
| 8 | 3.054 | -3.910 | 3.830 | | | | |
| 8 | 0.987 | -2.334 | 3.146 | | | | |
| 1 | 3.213 | -4.766 | 4.240 | | | | |
| 1 | 2.766 | -1.332 | 3.489 | | | | |
| 1 | 1.802 | -3.477 | 5.436 | | | | |
| 1 | 3.389 | -2.650 | 5.456 | | | | |
| 1 | 2.242 | -0.665 | 6.708 | | | | |
| 1 | 0.523 | -1.283 | 5.570 | | | | |
| 1 | 1.335 | 0.653 | 3.370 | | | | |
| 1 | -2.125 | 0.491 | 2.182 | | | | |
| 1 | -0.537 | -0.507 | 2.531 | | | | |
| 1 | 1.386 | 1.416 | 5.691 | | | | |
| 1 | 1.376 | -3.128 | 2.752 | | | | |
| without catalyst – TS2 cis | | | | | | | |
| 6 | 0.567 | 0.017 | 2.563 | | | | |
| 8 | -0.187 | -0.682 | 3.306 | | | | |
| 6 | 0.533 | 0.071 | 1.106 | | | | |
| 6 | 1.674 | 0.831 | 0.419 | | | | |
| 6 | 1.141 | 1.593 | -0.799 | | | | |
| 6 | 2.209 | 2.426 | -1.492 | | | | |
| 8 | 2.701 | 3.366 | -0.549 | | | | |
| 8 | -0.308 | -0.557 | 0.381 | | | | |
| 8 | 2.672 | -0.105 | 0.025 | | | | |
| 8 | 0.628 | 0.660 | -1.735 | | | | |
| 6 | 1.662 | 3.152 | -2.707 | | | | |
| 8 | 2.724 | 3.969 | -3.190 | | | | |
| 1 | 1.454 | 0.533 | 2.984 | | | | |
| 1 | 2.370 | 4.612 | -3.812 | | | | |
| 1 | 3.024 | 1.761 | -1.817 | | | | |
| 1 | 0.804 | 3.771 | -2.411 | | | | |
| 1 | 1.339 | 2.430 | -3.465 | | | | |
| 1 | 0.066 | 0.067 | -1.173 | | | | |
| 1 | 0.347 | 2.275 | -0.449 | | | | |
| 1 | 2.151 | 1.528 | 1.114 | | | | |
| 1 | 0.044 | 1.124 | 1.967 | | | | |

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