Thermodynamics of Hydronium, Zundel and Eigen ions

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Abstract: The heterolytic dissociation of water gives the cation of proton, which has fleeting existence in reality. It exists in aqueous solution in various levels of hydration, as hydronium (H_3O^+), Zundel (H_5O_2^+) and Eigen (H_9O_4^+) ions. Herein, we present the thermodynamic parameters involved in the overall treatment. These values are crucial in understanding the behaviour of water and protons in cellular physiology at interfaces and bulk.

Keywords: proton; water; hydronium; Zundel ion; Eigen ion; solvation

The biological solvent of water has a low dissociation, and this is very important towards explaining several physiological activities. Herein, we present the values of thermodynamica constants for the various species, in continuing efforts to understand the dynamics of bioenergetics.

1. H_3O^+

1.1 The thermodynamic parameters for $\text{H}_2\text{O}_{\text{gas}}$ and H_{gas}^+

The used thermodynamic parameters for $\text{H}_2\text{O}_{\text{gas}}$ and H_{gas}^+ are taken from [1, 2]

Parameters H_3O^+ formation reaction in the gas phase are taken from [1, Table 10-168]:

1.2. The thermodynamic functions of the formation of $\text{H}_3\text{O}_{\text{gas}}^+$

Let us now find the values of the thermodynamic functions of the formation of ions $\text{H}_3\text{O}_{\text{gas}}^+$ in the gas phase. From the last equation ($\text{H}_2\text{O}_{\text{gas}} + \text{H}_{\text{gas}}^+ \rightarrow \text{H}_3\text{O}_{\text{gas}}^+$) we find

$$\begin{aligned} \Delta_r H^\circ &= \Delta_f H^\circ(\text{H}_3\text{O}_{\text{gas}}^+) - \Delta_f H^\circ(\text{H}_{\text{gas}}^+) - \Delta_f H^\circ(\text{H}_2\text{O}_{\text{gas}}) = \\ &-690.36 = \Delta_f H^\circ(\text{H}_3\text{O}_{\text{gas}}^+) - 1536.2 + 241.8 \end{aligned}$$

and

$$\Delta_f H^\circ(\text{H}_3\text{O}_{\text{gas}}^+) = -690.36 + 1536.2 - 241.8 = 604.04 \text{ kJ/mol}$$

Similarly, we find the values of the Gibbs function

$$\begin{aligned} \Delta_r G^\circ &= \Delta_f G^\circ(\text{H}_3\text{O}_{\text{gas}}^+) - \Delta_f G^\circ(\text{H}_{\text{gas}}^+) - \Delta_f G^\circ(\text{H}_2\text{O}_{\text{gas}}) = \\ &-660 = \Delta_f G^\circ(\text{H}_3\text{O}_{\text{gas}}^+) - 1517 + 228.6 \text{ and} \\ \Delta_f G^\circ(\text{H}_3\text{O}_{\text{gas}}^+) &= -660 + 1517 - 228.6 = 628.4 \text{ kJ/mol} \end{aligned}$$

1.3. Solvation

We will consider the process of solvation of a proton in the form of two reactions: the addition of a proton to a water molecule in the gas phase and the solvation of the formed ion $\text{H}_3\text{O}_{\text{gas}}^+$.

In the case of enthalpy we have

$$\Delta_s H^\circ(\text{H}^+) = \Delta_r H^\circ(\text{H}_2\text{O} + \text{H}^+)_{\text{gas}} + \Delta_s H^\circ(\text{H}_3\text{O}^+) = -690.36 + \Delta_s H^\circ(\text{H}_3\text{O}^+).$$

From the last equation we obtain

$$\Delta_s H^\circ (\text{H}_3\text{O}^+) = \Delta_s H^\circ (\text{H}^+) + 690.36 = -1150.1 + 690.36 = -459.74 \text{ kJ/mol}$$

Carrying out similar calculations for the Gibbs function,

$$\Delta_s G^\circ (\text{H}^+) = -1104.5 = \Delta_s G^\circ (\text{H}_3\text{O}^+) + \Delta_r G^\circ (\text{H}_2\text{O} + \text{H}^+) = \Delta_s G^\circ (\text{H}_3\text{O}^+) - 660.$$

we find

$$\Delta_s G^\circ (\text{H}_3\text{O}^+) = \Delta_s G^\circ (\text{H}^+) + 660 = -1104.5 + 660 = -444.5 \text{ kJ/mol}.$$

1.4. The thermodynamic parameters of $\text{H}_3\text{O}^+_{\text{aq}}$

Knowing the thermodynamic parameters of solvation and thermodynamic parameters in the gas phase we calculate the standard values of the thermodynamic parameters formation for $\text{H}_3\text{O}^+_{\text{aq}}$ in an aqueous solution.

$$\Delta_s H^\circ (\text{H}_3\text{O}^+) = \Delta_f H^\circ (\text{H}_3\text{O}^+_{\text{aq}}) - \Delta_f H^\circ (\text{H}_3\text{O}^+_{\text{gas}}) \text{ and}$$

$$\Delta_f H^\circ (\text{H}_3\text{O}^+_{\text{aq}}) = \Delta_s H^\circ (\text{H}_3\text{O}^+) + \Delta_f H^\circ (\text{H}_3\text{O}^+_{\text{gas}}) = -459.74 + 604.04 = 144.3 \text{ kJ/mol}$$

For G function we have

$$\Delta_s G^\circ (\text{H}_3\text{O}^+) = \Delta_f G^\circ (\text{H}_3\text{O}^+_{\text{aq}}) - \Delta_f G^\circ (\text{H}_3\text{O}^+_{\text{gas}}) \text{ and}$$

$$\Delta_f G^\circ (\text{H}_3\text{O}^+_{\text{aq}}) = \Delta_s G^\circ (\text{H}_3\text{O}^+) + \Delta_f G^\circ (\text{H}_3\text{O}^+_{\text{gas}}) = -444.5 + 628.4 = 183.9 \text{ kJ/mol}.$$

1.5. Transformed value

Transformed value is equal

$$\Delta_f G^{\circ} (\text{H}_3\text{O}^+_{\text{aq}}) = \Delta_f G^\circ (\text{H}_3\text{O}^+_{\text{aq}}) + 121.49[3] = 183.9 + 121.49 = 305.39 \text{ kJ/mol}$$

1.6. Convention values

Knowing the standard thermodynamic parameters of $\text{H}_3\text{O}^+_{\text{aq}}$ formation, we find similar values within the framework of the convention [2]

$$\Delta_f H^{\circ}_{\text{conv}} (\text{H}_3\text{O}^+_{\text{aq}}) = \Delta_f H^\circ (\text{H}_3\text{O}^+_{\text{aq}}) - 386.25 = 144.3 - 386.25 = -241.95 \text{ kJ/mol and}$$

$$\Delta_f G^{\circ}_{\text{conv}} (\text{H}_3\text{O}^+_{\text{aq}}) = \Delta_f G^\circ (\text{H}_3\text{O}^+_{\text{aq}}) - 412.5 = 183.9 - 412.5 = -228.6 \text{ kJ/mol}$$

2. Zundel ion

2.1. The thermodynamic parameters for H_5O_2^+

Zundel ion is $\text{H}_5\text{O}_2^+ = \text{H}^+ \dots 2\text{H}_2\text{O}$.

We write the formation of an Zundel ion in gas phase in the form of two reactions

From [4], we take data from Table 1

Table I. Experimental Thermodynamic Values for the Gas-Phase Reactions

(n - 1, n)	$-\Delta H_{n-1,n}$ kcal/mol	$-\Delta H_{n-1,n}$ kJ/mol	$-\Delta G_{n-1,n}$ kcal/mol	$-\Delta G_{n-1,n}$ kJ/mol
0,1	165	690.36		660 [1]
1,2	36	150.62	25	104.6
2,3	22.3	93.3	13.6	56.9
3,4	17	71.13	8.5	35.56

Hence, $\Delta_r H(\text{H}^+ + 2 \text{H}_2\text{O} \rightarrow \text{H}_5\text{O}_2^+)_{\text{gas}} = -690.36 - 150.62 = -840.98 \text{ kJ/mol}$ and

$$\Delta_r G(\text{H}^+ + 2 \text{H}_2\text{O} \rightarrow \text{H}_5\text{O}_2^+)_{\text{gas}} = -660 - 104.6 = -764.6 \text{ kJ/mol}$$

2.2. The thermodynamic functions of H_5O_2^+

For the reaction of formation of H_5O_2^+ , $(\text{H}^+ + 2 \text{H}_2\text{O} \rightarrow \text{H}_5\text{O}_2^+)_{\text{gas}}$, we write

$$\begin{aligned} \Delta_r H^\circ &= \Delta_f H^\circ(\text{H}_5\text{O}_2^+) - \Delta_f H^\circ(\text{H}_{\text{gas}}^+) - 2 \Delta_f H^\circ(\text{H}_2\text{O}_{\text{gas}}) = \\ &= -840.98 = \Delta_f H^\circ(\text{H}_5\text{O}_2^+) - 1536.2 + 2 \cdot 241.8 \text{ and} \end{aligned}$$

Hence

$$\Delta_f H^\circ(\text{H}_5\text{O}_2^+) = -840.98 + 1536.2 - 2 \cdot 241.8 = 211.62 \text{ kJ/mol}$$

Similarly, we find the values of the Gibbs function

$$\begin{aligned} \Delta_r G^\circ &= \Delta_f G^\circ(\text{H}_5\text{O}_2^+) - \Delta_f G^\circ(\text{H}_{\text{gas}}^+) - 2 \cdot \Delta_f G^\circ(\text{H}_2\text{O}_{\text{gas}}) = \\ &= -764.6 = \Delta_f G^\circ(\text{H}_5\text{O}_2^+) - 1517 + 2 \cdot 228.6 \text{ and} \end{aligned}$$

$$\Delta_f G^\circ (\text{H}_5\text{O}_2^+_{\text{gas}}) = -764.6 + 1517 - 2 \cdot 228.6 = 295.2 \text{ kJ/mol}$$

2.3. Solvation

We will consider the process of solvation of a proton in the form of two reactions: the addition of a proton to a two water molecules in the gas phase and the solvation of the formed ion H_5O_2^+ .

In the case of enthalpy we have

$$\Delta_S H^\circ (\text{H}^+) = \Delta_r H^\circ (\text{H}^+ + 2\text{H}_2\text{O})_{\text{gas}} + \Delta_S H^\circ (\text{H}_5\text{O}_2^+) = -840.98 + \Delta_S H^\circ (\text{H}_5\text{O}_2^+).$$

From the last equation we obtain

$$\Delta_S H^\circ (\text{H}_5\text{O}_2^+) = \Delta_S H^\circ (\text{H}^+) + 840.98 = -1150.1 + 840.98 = -309.12 \text{ kJ/mol}$$

Carrying out similar calculations for the Gibbs function,

$$\Delta_S G^\circ (\text{H}^+) = -1104.5 = \Delta_r G^\circ (\text{H}^+ + 2 \text{H}_2\text{O} \rightarrow \text{H}_5\text{O}_2^+)_{\text{gas}} + \Delta_S G^\circ (\text{H}_5\text{O}_2^+) = \Delta_S G^\circ (\text{H}_5\text{O}_2^+) - 764.6 \text{ kJ/mol}.$$

we find

$$\Delta_S G^\circ (\text{H}_5\text{O}_2^+) = -1104.5 + 764.6 = -333.9 \text{ kJ/mol}.$$

2.4. The thermodynamic parameters of H_5O_2^+

Knowing the thermodynamic parameters of solvation and thermodynamic parameters in the gas phase we calculate the standard values of the thermodynamic parameters formation for H_5O_2^+ in an aqueous solution.

$$\Delta_S H^\circ (\text{H}_5\text{O}_2^+) = \Delta_f H^\circ (\text{H}_5\text{O}_2^+_{\text{aq}}) - \Delta_f H^\circ (\text{H}_5\text{O}_2^+_{\text{gas}}) \text{ and}$$

$$\Delta_f H^\circ (\text{H}_5\text{O}_2^+_{\text{aq}}) = \Delta_S H^\circ (\text{H}_5\text{O}_2^+) + \Delta_f H^\circ (\text{H}_5\text{O}_2^+_{\text{gas}}) = -309.12 + 211.62 = -97.5 \text{ kJ/mol}$$

For G function we have

$$\Delta_S G^\circ (\text{H}_5\text{O}_2^+) = \Delta_f G^\circ (\text{H}_5\text{O}_2^+_{\text{aq}}) - \Delta_f G^\circ (\text{H}_5\text{O}_2^+_{\text{gas}}) \text{ and}$$

$$\Delta_f G^\circ (\text{H}_5\text{O}_2^+_{\text{aq}}) = \Delta_S G^\circ (\text{H}_5\text{O}_2^+) + \Delta_f G^\circ (\text{H}_5\text{O}_2^+_{\text{gas}}) = -333.9 + 295.2 = -38.7 \text{ kJ/mol}$$

2.5. Transformed value

Transformed value is equal

$$\Delta_f G^\circ (\text{H}_5\text{O}_2^+_{\text{aq}}) = \Delta_f G^\circ (\text{H}_5\text{O}_2^+_{\text{aq}}) + 121.49 [3] = -38.7 + 203.03 = 164.33 \text{ kJ/mol}$$

2.6. Convention values

Knowing the standard thermodynamic parameters of $\text{H}_5\text{O}_2^+_{\text{aq}}$ formation, we find similar values within the framework of the convention

$$\Delta_f H^\circ_{\text{conv}}(\text{H}_5\text{O}_2^+_{\text{aq}}) = \Delta_f H^\circ(\text{H}_5\text{O}_2^+_{\text{aq}}) - 386.25 = -97.5 - 386.25 = -483.75 \text{ kJ/mol and}$$

$$\Delta_f G^\circ_{\text{conv}}(\text{H}_5\text{O}_2^+_{\text{aq}}) = \Delta_f G^\circ(\text{H}_5\text{O}_2^+_{\text{aq}}) - 412.5 = -38.7 - 412.5 = -451.2 \text{ kJ/mol}$$

3. Eigen ion

Eigen ion is $\text{H}_9\text{O}_4^+ = \text{H}^+ \dots 4\text{H}_2\text{O}$

2.1. The thermodynamic parameters for $\text{H}_9\text{O}_{4\text{gas}}^+$

Eigen ion is $\text{H}_5\text{O}_2^+ = \text{H}^+ \dots 2\text{H}_2\text{O}$.

We write the formation of an Eigen ion in gas phase in the form of fourth reactions

Hence, $\Delta_f H(\text{H}^+ + 4 \text{H}_2\text{O} \rightarrow \text{H}_9\text{O}_4^+)_{\text{gas}} = -690.36 - 150.62 - 93.3 - 71.13 = -1005.41 \text{ kJ/mol and}$

$$\Delta_f G(\text{H}^+ + 4 \text{H}_2\text{O} \rightarrow \text{H}_9\text{O}_4^+)_{\text{gas}} = -660 - 104.6 - 56.9 - 35.56 = -857.06 \text{ kJ/mol}$$

3.2. The thermodynamic functions of $\text{H}_9\text{O}_{4\text{gas}}^+$

For the reaction of formation of $\text{H}_9\text{O}_{4\text{gas}}^+$, $(\text{H}^+ + 4 \text{H}_2\text{O} \rightarrow \text{H}_9\text{O}_4^+)$, we write

$$\begin{aligned}
 \Delta_f H^\circ &= \Delta_f H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) - \Delta_f H^\circ(\text{H}_{\text{gas}}^+) - 4 \Delta_f H^\circ(\text{H}_2\text{O}_{\text{gas}}) = \\
 -1005.41 &= \Delta_f H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) - 1536.2 + 4 \cdot 241.8
 \end{aligned}$$

Hence

$$\Delta_f H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) = -1005.41 + 1536.2 - 4 \cdot 241.8 = -436.41 \text{ kJ/mol}$$

Similarly, we find the values of the Gibbs function

$$\begin{aligned}\Delta_r G^\circ &= \Delta_f G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) - \Delta_f G^\circ(\text{H}_{\text{gas}}^+) - 4 \cdot \Delta_f G^\circ(\text{H}_2\text{O}_{\text{gas}}) = \\ &- 857.06 = \Delta_f G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) - 1517 + 4 \cdot 228.6 \quad \text{and} \\ \Delta_f G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) &= -857.06 + 1517 - 4 \cdot 228.6 = -254.46 \text{ kJ/mol}\end{aligned}$$

3.3. Solvation

We will consider the process of solvation of a proton in the form of two reactions: the addition of a proton to a fourth water molecules in the gas phase and the solvation of the formed ion $\text{H}_9\text{O}_{4\text{gas}}^+$.

In the case of enthalpy we have

$$\Delta_S H^\circ(\text{H}^+) = \Delta_r H^\circ(\text{H}^+ + 4\text{H}_2\text{O})_{\text{gas}} + \Delta_S H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) = -1005.41 + \Delta_S H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+).$$

From the last equation we obtain

$$\Delta_S H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) = \Delta_S H^\circ(\text{H}^+) + 1005.41 = -1150.1 + 1005.41 = -144.69 \text{ kJ/mol}$$

Carrying out similar calculations for the Gibbs function,

$$\begin{aligned}\Delta_S G^\circ(\text{H}^+) &= -1104.5 = \Delta_r G^\circ(\text{H}^+ + 4\text{H}_2\text{O} \rightarrow \text{H}_9\text{O}_{4\text{gas}}^+)_{\text{gas}} + \Delta_S G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) = \\ &\Delta_S G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) - 857.06 \text{ kJ/mol}.\end{aligned}$$

we find

$$\Delta_S G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) = -1104.5 + 857.06 = -247.44 \text{ kJ/mol}.$$

3.4. The thermodynamic parameters of $\text{H}_9\text{O}_{4\text{aq}}^+$

Knowing the thermodynamic parameters of solvation and thermodynamic parameters in the gas phase we calculate the standard values of the thermodynamic parameters formation for $\text{H}_9\text{O}_{4\text{aq}}^+$ in an aqueous solution.

$$\Delta_S H^\circ(\text{H}_9\text{O}_4^+) = \Delta_f H^\circ(\text{H}_9\text{O}_{4\text{aq}}^+) - \Delta_f H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) \text{ and}$$

$$\Delta_f H^\circ(\text{H}_9\text{O}_{4\text{aq}}^+) = \Delta_S H^\circ(\text{H}_9\text{O}_4^+) + \Delta_f H^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) = -144.69 - 436.41 = -581.1 \text{ kJ/mol}$$

For G function we have

$$\Delta_S G^\circ(\text{H}_9\text{O}_4^+) = \Delta_f G^\circ(\text{H}_9\text{O}_{4\text{aq}}^+) - \Delta_f G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) \text{ and}$$

$$\Delta_f G^\circ(\text{H}_9\text{O}_{4\text{aq}}^+) = \Delta_S G^\circ(\text{H}_9\text{O}_4^+) + \Delta_f G^\circ(\text{H}_9\text{O}_{4\text{gas}}^+) = -247.44 - 254.46 = -501.9 \text{ kJ/mol}$$

3.5. Transformed value

Transformed value is equal

$$\Delta_f G^{\circ}(\text{H}_9\text{O}_{4\text{aq}}^+) = \Delta_f G^{\circ}(\text{H}_9\text{O}_{4\text{aq}}^+) + 366.09 [3] = -501.9 + 366.09 = -135.81 \text{ kJ/mol}$$

3.6. Convention values

Knowing the standard thermodynamic parameters of $\text{H}_9\text{O}_{4\text{aq}}^+$ formation, we find similar values within the framework of the convention

$$\Delta_f H_{\text{conv}}^{\circ}(\text{H}_9\text{O}_{4\text{aq}}^+) = \Delta_f H^{\circ}(\text{H}_9\text{O}_{4\text{aq}}^+) - 386.25 = -581.1 - 386.25 = -967.35 \text{ kJ/mol and}$$

$$\Delta_f G_{\text{conv}}^{\circ}(\text{H}_9\text{O}_{4\text{aq}}^+) = \Delta_f G^{\circ}(\text{H}_9\text{O}_{4\text{aq}}^+) - 412.5 = -501.9 - 412.5 = -914.4 \text{ kJ/mol}$$

4.1 Cation $\text{H}_{17}\text{O}_8^+$

4.1. The thermodynamic parameters for $\text{H}_{17}\text{O}_8^+$

Hence due to [4], $\Delta_r H(\text{H}^+ + 8 \text{H}_2\text{O} \rightarrow \text{H}_{17}\text{O}_8^+) = -1215.87 \text{ kJ/mol}$ and

$$\Delta_r G = -917.32 \text{ kJ/mol}$$

4.2. The thermodynamic functions of $\text{H}_{17}\text{O}_8^+$

For the reaction of formation of $\text{H}_{17}\text{O}_{8\text{gas}}^+$, we write

$$\begin{aligned} \Delta_r H^{\circ} &= \Delta_f H^{\circ}(\text{H}_{17}\text{O}_8^+) - \Delta_f H^{\circ}(\text{H}_{\text{gas}}^+) - 8 \Delta_f H^{\circ}(\text{H}_2\text{O}_{\text{gas}}) = \\ &= -1215.87 = \Delta_f H^{\circ}(\text{H}_{17}\text{O}_{8\text{gas}}^+) - 1536.2 + 8 \cdot 241.8 \end{aligned}$$

Hence

$$\Delta_f H^{\circ}(\text{H}_{17}\text{O}_{8\text{gas}}^+) = -1215.87 + 1536.2 - 8 \cdot 241.8 = -1614.07 \text{ kJ/mol}$$

Similarly, we find the values of the Gibbs function

$$\begin{aligned} \Delta_r G^{\circ} &= \Delta_f G^{\circ}(\text{H}_{17}\text{O}_8^+) - \Delta_f G^{\circ}(\text{H}_{\text{gas}}^+) - 4 \cdot \Delta_f G^{\circ}(\text{H}_2\text{O}_{\text{gas}}) = \\ &= -917.32 = \Delta_f G^{\circ}(\text{H}_{17}\text{O}_{8\text{gas}}^+) - 1517 + 8 \cdot 228.6 \quad \text{and} \\ \Delta_f G^{\circ}(\text{H}_{17}\text{O}_{8\text{gas}}^+) &= -917.32 + 1517 - 8 \cdot 228.6 = -1229.12 \text{ kJ/mol} \end{aligned}$$

4.3. Solvation

We will consider the process of solvation of a proton in the form of two reactions: the addition of a proton to a 8 water molecules in the gas phase and the solvation of the formed ion $H_{17}O_{8gas}^+$.

In the case of enthalpy we have

$$\Delta_S H^o(H^+) = \Delta_r H^o(H^+ + 8H_2O)_{gas} + \Delta_S H^o(H_{17}O_{8gas}^+) = -1215.87 + \Delta_S H^o(H_{17}O_{8gas}^+).$$

From the last equation we obtain

$$\Delta_S H^o(H_{17}O_{8gas}^+) = \Delta_S H^o(H^+) + 1215.87 = -1150.1 + 1215.87 = +65.77 \text{ kJ/mol}$$

Summation:

N o	Ion	$\Delta_f H_{gas}^o$ kJ/mol	$\Delta_f G_{gas}^o$ kJ/mol	$\Delta_S H^o$ kJ/mol	$\Delta_S G^o$ kJ/mol	$\Delta_f H_{aq}^o$ kJ/mol	$\Delta_f G_{aq}^o$ kJ/mol	$\Delta_f G_{aq}^{io}$ J/mol	$\Delta_f H_{aq}^{o \text{ conv}}$ kJ/mol	$\Delta_f G_{aq}^{o \text{ conv}}$ kJ/mol
1	H^+	1536.2	1517	-1150.1	-1104.5	386.25	412.5	452.46	0	0
2	H_3O^+	604.04	628.4	-459.74	-444.5	144.3	183.9	305.39	-241.95	-228.6
3	$H_5O_2^+$	211.62	295.2	-309.12	-333.9	-97.5	-38.7	164.33	-483.75	-451.2
4	$H_9O_4^+$	-436.41	-254.46	-144.69	-247.44	-581.1	-501.9	-135.81	-967.35	-914.4
5	$H_{17}O_8^+$	-1614.07	-1229.12	+65.77						

The parameters for H^+ are taken from [2].

Thermodynamic functions in the convention version were calculated in accordance with [2]

$$\Delta_f H_{aq}^{o \text{ conv}} = \Delta_f H_{aq}^o - 386.25 \text{ kJ/mol} \quad \Delta_f G_{aq}^{o \text{ conv}} = \Delta_f G_{aq}^o - 412.5 \text{ kJ/mol}$$

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