Visualization of Chemical Reactions for Teaching Material Based on Quantum Calculation – Thermochemical Handling about NaCl

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Abstract: Original Born-Haber cycle about sodium chloride NaCl is proposed as a teaching material based on the calculation result by the quantum calculation with MOPAC MP6 Hamiltonian level. Enthalpy changes of the corresponding processes *via* NaCl-related substances on the basis of the formation energies are depicted in the cycle. Furthermore, the intelligible diagram about dissolution phenomenon is carried out by the thermodynamic changes of enthalpy, entropy and Gibbs function for student to understand meaning of the thermodynamic changes in the phenomenon.

Keywords: Visualization, quantum calculation, thermochemistry, teaching material Born-Haber cycle of NaCl

Introduction

The learning on the basis of students' enthusiastic activities on imaginative thinking and behaving would be of great importance to understand science. Student's attitude being enthusiastic toward the possibilities of their own abilities with their own images would enhance the understanding of objectives. Dividing the lecture stage into the three thinking levels is mentioned by Tasker *et al* [1]. Visualization as a key of representation of images is great help for student to have images of phenomena, chemical concepts, and molecular world, and then the visualization enables student to realize images of them. Visualization of chemical abstract concepts on CG graphics helps us greatly to realize images of them, and the visualization is one of effective methodologies for making teaching material [2]. The visualization needs to be more appealing for students from the stand point of a useful teaching material. It is our aim to produce a teaching material in accordance with this manner [3, 4].

Born-Haber cycle related with sodium chloride NaCl is well known thermodynamic procedure for student's learning of theromochemistry [5]. An understanding of thermodynamics tends to be unclear and tends to have misunderstanding. For example, if the dissolution phenomenon of salt is taken, the dissolution will take place spontaneously thermodynamically with a value positive in enthalpy change, and then an understanding of a relation with entropy change will become ambiguous easily. This paper reports the study on thermochemical teaching material by quantum calculation in which original Born-Haber cycle related with sodium chloride NaCl is established for student to understand meaning of the thermodynamic changes in the phenomenon.

1. Procedure

The semi-empirical molecular orbital calculation software *MOPAC* in the *CAChe Work System for Windows ver. 5.04* (Fujitsu, Inc.) with PM6 Hamiltonian was used in calculations for optimization of heat of formation $\varDelta E_f$ as origin. The $\varDelta E_f$ was calculated on the basis of the definition of heat of formation ($E_{elect} + E_{nuc} - E_{isol} + E_{atom}$) [6].
Enthalpy changes $\varDelta H$ of the corresponding processes were calculated on the basis of the $\varDelta E_f$. $\varDelta H_{dissol}$ of the dissolution process of NaCl(s) → NaCl(aq) was estimated by our practical data from the experiment of NaCl dissolution in water at 298 K.

2. Results and Discussion

2.1 Born-Haber Cycle

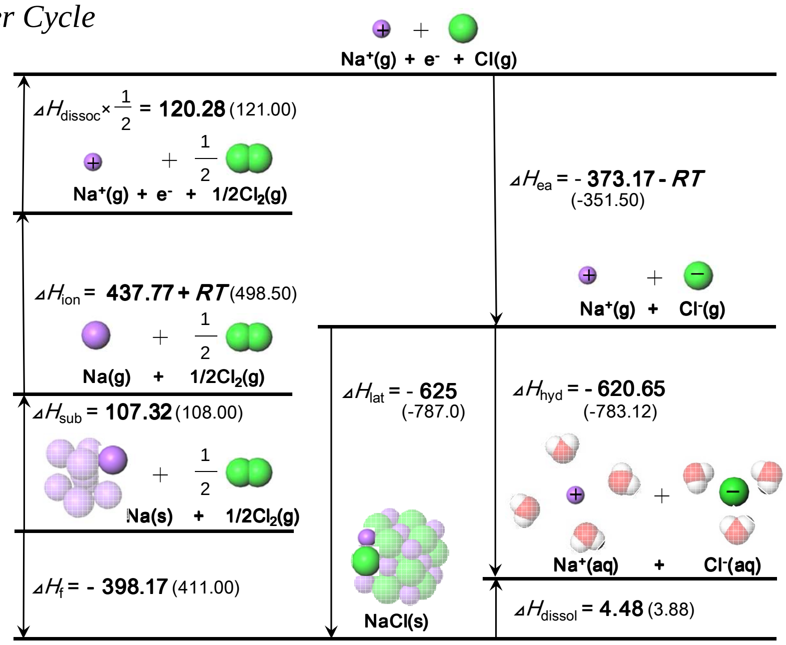

Fig. 1. Born-Haber cycle[a]

[a] $\triangle H$ / kJmol^{-1} is calculated from $\triangle E_f$; $\triangle H_{dissol}$ was estimated from our experiment of NaCl dissolution in water at 298 K. Vales inside of a parenthesis are cited in the reference [7].

Calculated heat of formation $\varDelta E_f$ / kJmol^{-1} as an original of NaCl-related species were as follows; –206.67 as NaCl(g), 107.32 as Na(g), 121.15 as Cl(g), 545.09 as Na^+(g), –252.02 as Cl^- (g), –1.74 as Cl_2(g), and –331.98 as NaCl(s). Enthalpy changes $\varDelta H$ among steps in the reaction process related with NaCl are able to find out from the combination of $\varDelta E_f$.
Calculated $\varDelta H$ is represented in Fig. 1 as an original Born-Haber cycle, with definition of subscription of f: formation, sub: sublimation, ion: ionization, dissoc: dissociation, ea: electron affinity, hyd: hydration, dissol: dissolution, lat: lattice with reference value inside of a parenthesis [7]. For the purpose of clear stoichiometry, state of molecule with relative size is represented. We should use the ionization enthalpy, $\varDelta H_{ion} + RT$, $\varDelta \nu_{gas} = +1$ and enthalpy of electron affinity, $\varDelta H_{ea} + RT$, $\varDelta \nu_{gas} = -1$; but not only is the difference small (RT = 2.5 kJmol^{-1} at 298 K), the RT is in fact cancelled by a similar term mentioned above.

2.2 Dissolution

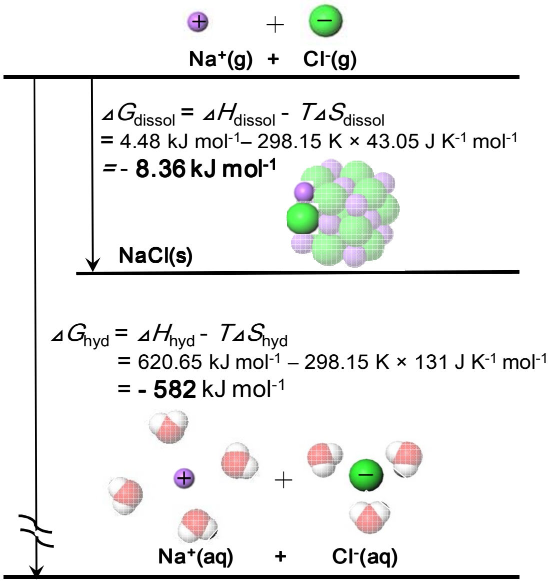

Fig. 2. Dissolution

An intelligible diagram about dissolution phenomenon is advocated in Fig. 2 with the thermodynamic changes of enthalpy, entropy and Gibbs function in order that student may understand the meaning of thermodynamic changes in the phenomenon and treat thermochemical procedure with calculation by thermodynamic quantities. It is clear that dissolution phenomenon proceeds spontaneously even with the plus value of ΔH_{dissol} besides with plus value of ΔS_{dissol}, totally with minus value of ΔG_{dissol}. The visualization based on outcomes from the calculation would have strong possibility for teaching material to a smooth understanding for student to realize the whereabouts of the reaction.

References

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