Chapter 1

Introductory Chapter: Mathematical or Theoretical Treatments in Chemical Studies on Fire Materials

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Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/intechopen.74202

1. Introduction

This book entitled *Symmetry (Group Theory) and Mathematical Treatment in Chemistry* deals with not only basic mathematics associated with linear algebra and group theory describing chemical symmetry about not only molecular shapes, molecular orbitals, and crystal structures but also spectroscopic discussion, DFT calculations or other computational treatments of several molecules or supramolecules, and symmetric structures of formula used in thermodynamics. In this way, this aspect may be one of the important approaches in chemical studies (along hierarchical structures group theory) [1] describing.

2. Results and discussion

Herein, as an example, a study on fire materials and possibility to apply these approaches is mentioned. The flame retardants prevent the burning of the material by either cutting the air supply or enhancing the requirements of oxygen. Some of the flame retardant used in the PVC or polymers can be classified as follows: (a) phosphorous compounds, (b) halogen compounds, (c) halogen phosphorous compounds, and (d) bicarbonates and inorganic oxides and borates. Some of the flame retardants may be broadly classified as halogen, and the aim of this example study is to prepare brominated (potential flame retardants) metal complexes to use as DSSC dyes, too. Crystal structure (space group $P2_1$) of a brominated complex (**Figure 1**) [2] is relative to crystal symmetry as condensed solid states or supramolecules. With the aid of DFT calculations [3], electronic states (UV-vis spectra) due to each transition between orbitals (of a certain irreducible representation) of the related complexes (**Figure 2**) could be estimated based on optimized molecular structures (coordination geometry is approximately $C2_v$). Of course, their

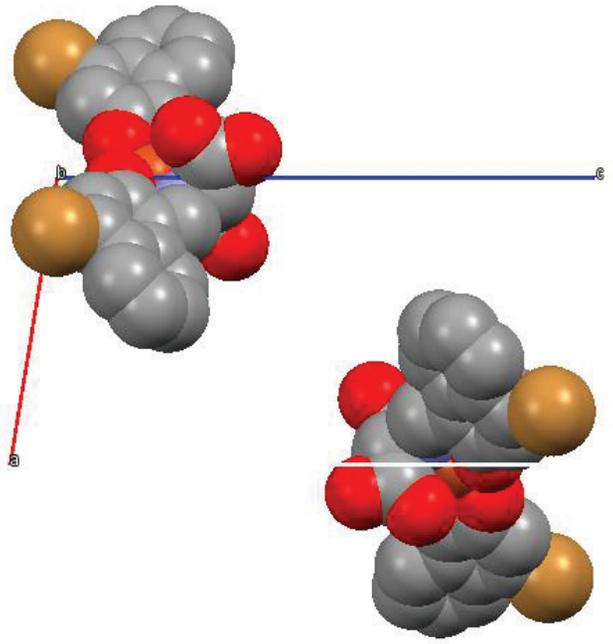

Figure 1. Crystal structure of a chiral complex.

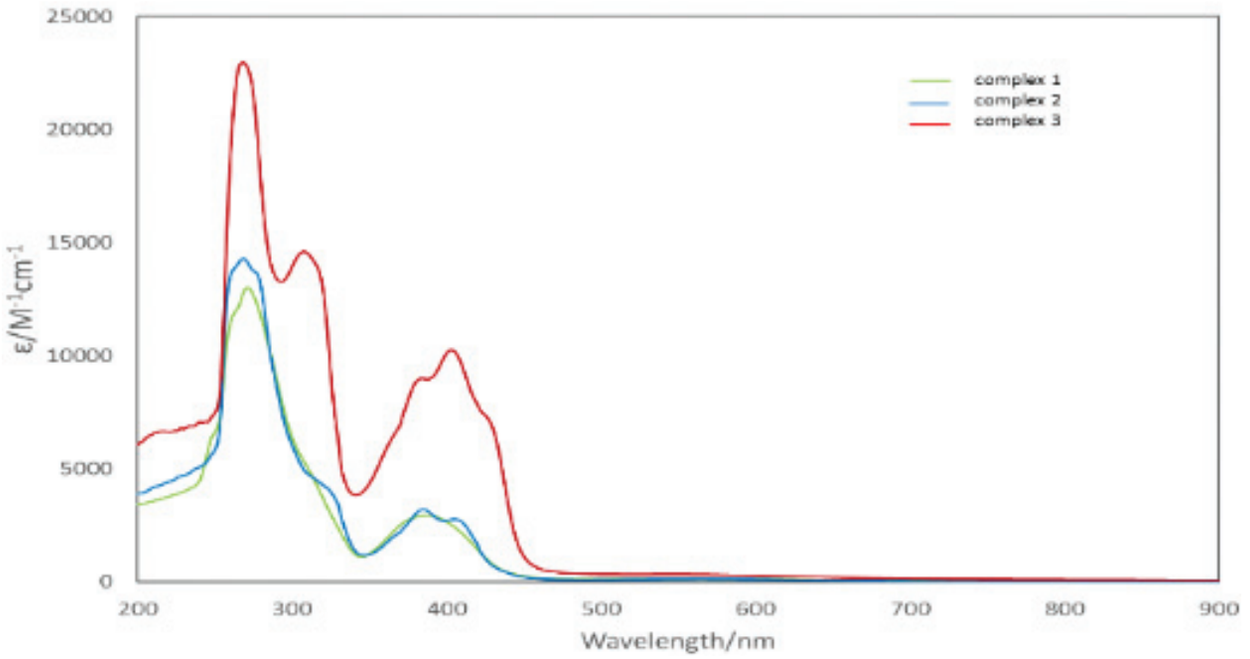

Figure 2. Electronic spectra.

vibrational (commonly infrared) spectra with normal modes (**Figure 3**) were relevant to molecular symmetry.

However, TG-DTA (**Figure 4**), a typical thermal analysis with "temperature" of crystalline complexes as well as hybrid materials dispersed in several types of polymer films was less

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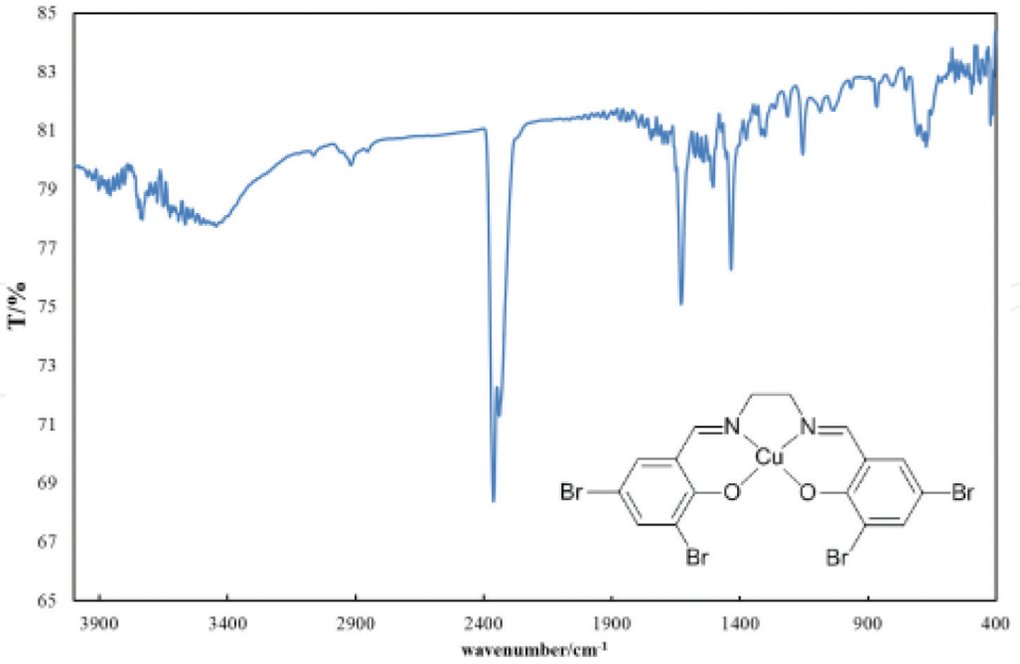

Figure 3. IR spectra (with structure).

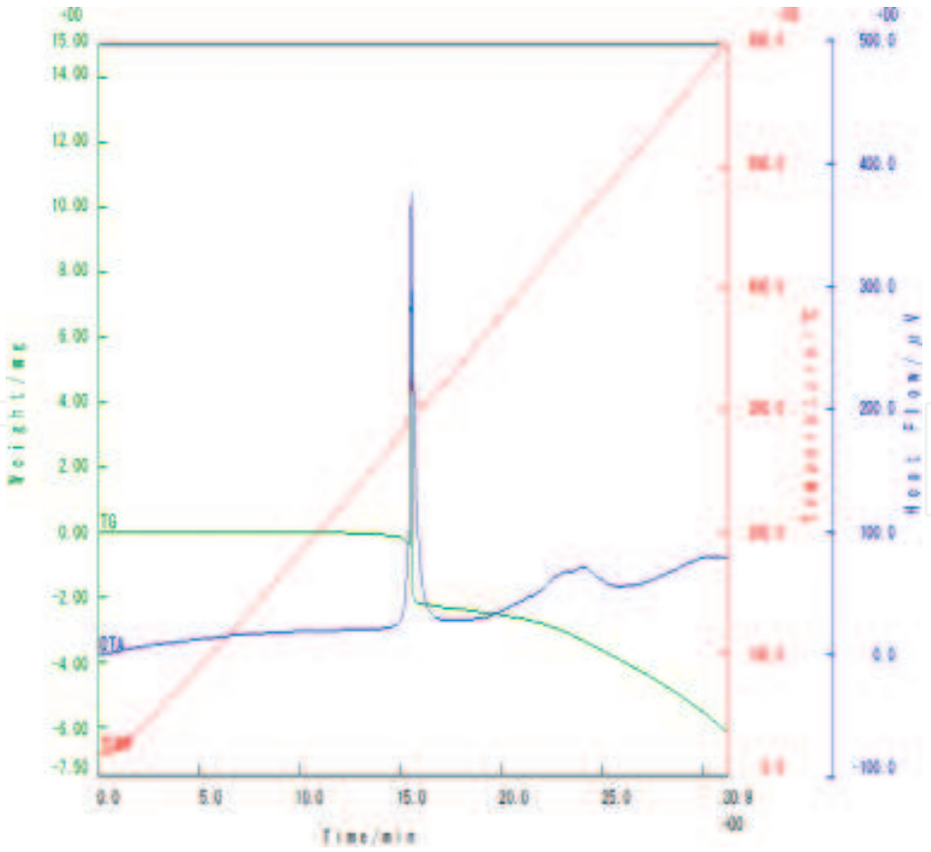

Figure 4. TG-DTA.

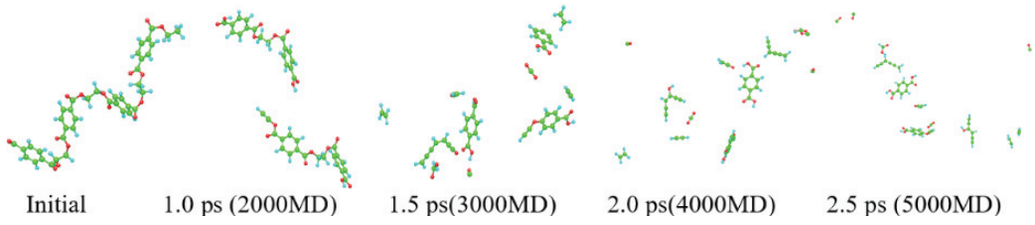

Figure 5. Thermolysis step of the quantity of PET polymer by the quantum molecular dynamics calculation.

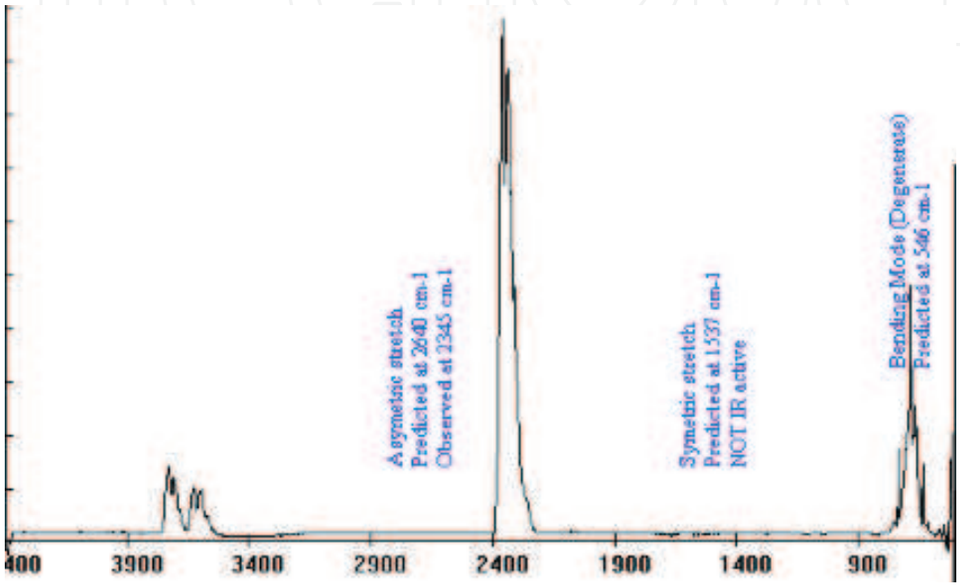

Figure 6. IR spectra of CO_2. The fundamental vibrations of molecules belonging to the $D_{\infty h}$ point group are similar in type to those of the nonsymmetrical linear molecules, but in this instance, they may also be symmetric (ν_s) or antisymmetric (ν_{as}) to the center of symmetry, and thus σ_g, σ_u, π_g, and π_u modes, two stretching and two bending (degenerate) vibrations. The ν_{as}(CO) mode and the degenerate δ(OCO) mode involve changes in the dipole moment during the vibration, and they are IR active. Thus, ν_{as} has been observed by IR as a very strong parallel-type band at 2349.3 cm^{-1}, while δ(OCO) appears as a strong perpendicular-type band at 667.3 cm^{-1}.

relevant to merely molecular symmetry. Furthermore, chemical reactions changing chemical species accompanying with "time" may be difficult to understand within the framework of symmetry. To discuss time-dependent chemical reaction, molecular dynamics may be a useful theoretical method of recently developed computations (**Figure 5**), while spectral detection of product gases (**Figure 6**) is sometimes possible to investigate closely rather than materials of solid states.

3. Conclusion

In this way, mathematical treatments of symmetry in chemistry can often lead to deep understanding, though it sometimes is not useless depending on conditions or phenomenon of targets. Similarly, theoretical computation should be carried out considering their limitation and frameworks (presupposition of theory).

http://dx.doi.org/10.5772/intechopen.74202

Acknowledgements

The author thanks Mrs. Keita Takahashi, Marin Yamaguchi, Shinosuke Tanaka, Kazuya Takakura; Profs. Mutsumi Sugiyama, Masayuki Mizuno, Ken Matsuyama, Kazunaka Endo (Tokyo University of Science); and Prof. Tomonori Ida (Kanazawa University), Prof. Mauricio Alcolea Palafox (Universidad Complutense de Madrid), and Prof. Rakesh Kumar Soni (Chaudhary Charan Singh University) for providing examples of studies.

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