Development of ConfDatMaker Software for Generating the Conformers of Metal Complexes

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ConfDatMaker software was developed for the purpose of generating the conformers of metal complexes. The software builds structures by symmetry operation of the inputted ligand coordinates, on the basis of the prepared enumeration results. A series of generated structures are useful for the conformational analysis.

Keywords: Conformer, Metal complex, Symmetry operation, Enumeration, ConfDatMaker software

1 INTRODUCTION

For conducting conformational analysis, enumeration of the full conformer set is necessary. In the case of metal complexes, the coordination numbers are larger than those of organic compounds. Therefore, the number of conformers for the metal complexes is generally much larger than that for the organic compounds. Enumeration of the conformers has been recently conducted for some octahedral metal complexes on the basis of computational group theory method [1–5]. On the other hand, however, it is not so easy to generate the structures of conformers from the result of enumeration. Therefore, the ConfDatMaker software has been developed for the purpose of generating the structures of conformers.

2 BASIC CONCEPTS

Let us consider a complex [M(AB)₆], where M is the central metal ion and AB is the diatomic ligand possessing atom A as the donor atom (Figure 1). The central MA₆ unit is assumed to belong to the O₅ point group. This complex has six AB ligands, and the bending angles of the six ligands are assumed to be the same but not to be equal to zero. By the combination of the ligand orientations around the M-A coordination bonds, the complex is expected to have numerous conformers. Here, we consider only two typical directions (Figure 2): (1) the edge-orientated direction, in which the B atom is oriented along the edge of the MA₆ octahedral geometry and (2) the bisecting direction, in which the B atom is oriented along the bisecting direction of the octahedral geometry.

The enumeration results were previously reported for the [M(AB)₆] complex [1,2], and the results are useful for generating the structures of conformers. Enumeration has been conducted also for some other types of metal complexes, including [M(ABC)₆] [3,5] and [MX(AB)₅] [4], and the enumeration results are increasing.

3 METHOD

The software was developed using Xojo software (2018 Release 1.1) [6] on a DELL Latitude 3570 computer (OS: Windows 10).

4 INPUT FOR CONFDATMAKER SOFTWARE

A set of atomic coordinates of the ligand and the code name for the conformer are necessary as input. For some ligands, a set of coordinates can be automatically given by one-click. An original set of coordinates can be manually introduced for other ligands. The code names of the conformers are included in the enumeration results. The bending angle, the M-L distance, and the central metal element can be optionally changed.

5 EXAMPLE OF OUTPUT

As an example, structures of conformers were generated for [VO(dmso)₅]⁺ complex cation [7], where dmso represents dimethyl-sulfoxide. For simplicity, we considered bisecting conformers of
[MX(AB)_5] type complex. By choosing the “dmsop” ligand and by inputting the code name “L5B1,” the 35 structures are automatically generated. The resulting structures are described in Figure 3, using the Winmostar software [8].

6 REQUIREMENTS

The software (ConfDatMaker) will run on Windows computers.

**Figure 2.** Edge-oriented directions (left) and bisecting directions (right) from an apex of an octahedron.

**Figure 3.** Bisecting diastereomers B1-B35 for [VO (dmsop)_5]^{2+} complex cation. Methyl groups are omitted for clarity.
7 CONCLUDING REMARKS

The ConfDatMaker software has been developed for the purpose of generating the conformer structures of metal complexes. The resulting structures are useful in conformational analysis. The software contains the library of the enumeration results, which is extending.

8 DISTRIBUTION

Information about distribution of the ConfDatMaker program will be given on the ResearchGate page of the author (https://www.researchgate.net/profile/Hiroshi_Sakiyama/).

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