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Enumeration of Edge-Orienting Conformers for Octahedral $[MX_{6-n}(AB_2)_n]$ Complexes (n = 1–5)

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Abstract

Edge-orienting conformers of octahedral $[MX_{6-n}(AB_2)_n]$ (n = 1 – 5) complexes have been enumerated on the basis of the group theory method, where M, X, and AB_2 are the central metal atom, monoatomic ligand, and the symmetrical triatomic ligand with a donor atom A, respectively. In the complexes, each MAB_2 unit is assumed to belong to the local C_{2v} point group. Since the enumeration had already been conducted for the $[M(AB_2)_6]$ complex, in this study, the enumeration was conducted for the following complexes: $[MX(AB_2)_5]$, *cis*-$[MX_2(AB_2)_4]$, *trans*-$[MX_2(AB_2)_4]$, *fac*-$[MX_3(AB_2)_3]$, *mer*-$[MX_3(AB_2)_3]$ *cis*-$[MX_4(AB_2)_2]$ *trans*-$[MX_4(AB_2)_2]$, and $[MX_5(AB_2)]$. In all the cases, the completeness of the enumerations was confirmed on the basis of the orbit-stabilizer theorem.

1 Introduction

Flexible molecules can have various conformer structures, and the dominant species should be clarified for a better understanding of the properties. Prediction of conformers is difficult for flexible octahedral metal complexes, because of the multiple junctions at the metal centers. Fundamental enumeration studies and related works have been actively conducted for cubic symmetry [1–23], and the enumeration results are very helpful for conformational prediction of flexible metal complexes [23–27].

Enumeration of the conformers for octahedral metal complexes were previously conducted only with the AB and bent ABC type ligands (Figure 1) [17–22], but recently the enumeration was conducted also for an octahedral metal complex with six C_{2v}-symmetric AB_2 ligands (Figure 1c) [23]. This enumeration result was found to be useful for conformational prediction of $[M(py)_6]$ type complex [23], where M and py represent the central metal atom and the pyridine ligand, respectively. For the purpose of extending the targets to penta-pyridine complexes, tetra-pyridine complexes, etc., in this study, conformers of octahedral $[MX_{6-n}(AB_2)_n]$ ($n = 1 - 5$) complexes have been enumerated on the basis of the group theory method (X: monoatomic ligand). In the complexes, each MAB_2 unit is assumed to belong to the local C_{2v} point group. For the C_{2v}-symmetric AB_2 ligand, there are two typical orientations on the octahedral coordination geometry: edge orientation and bisecting orientation (Figure 2); however, only the edge-orienting conformers were considered in this study, because the edge-orienting T_h conformer was found to be the only species for the $[Mg(py)_6]^{2+}$ complex cation [23].

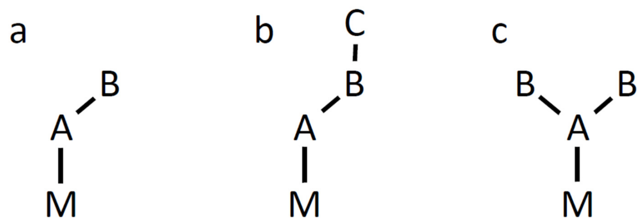

Figure 1. Three typical ligand moieties: an AB ligand in a bent form (a), a bent ABC ligand in a bent form (b), and a C_{2v}-symmetric AB_2 ligand (c).

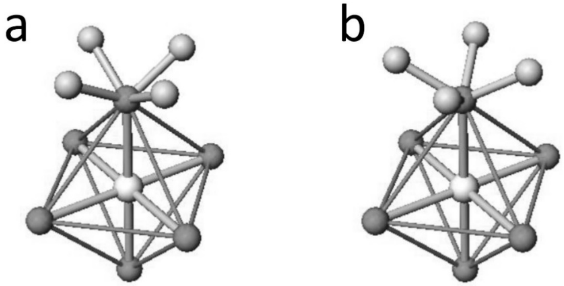

Figure 2. Typical orientations with respect to the octahedral coordination geometry: edge orientations (a) and bisecting orientations (b)

2 Methods

Three-dimensional models were handled by Winmostar software [28], and the point groups were confirmed by the software. The enumeration of the conformers was conducted on the basis of the group theory method. The enumeration algorithm is described in reference 29, and the enumeration was conducted manually. The completeness of enumerations was confirmed as follows. According to the orbit-stabilizer theorem [29], [the total number of each conformer] is equal to [the order of the rotation group of the conformer] divided by [the order of the rotation group of the coordination geometry], and the sum of the total number of each conformer should be equal to the number of structures (= 2^n for [$MX_{6-n}(AB_2)_n$] complex).

3 Results and discussion

3.1 Enumeration for octahedral [$MX(AB_2)_5$] complexes

The enumeration was conducted for the octahedral [$MX(AB_2)_5$] complex on the basis of the group theory. The conformers were exhaustively obtained without duplication by the algorithm according to the orbit-stabilizer theorem [29], and the resulting conformers are listed in Table 1, and their structures are depicted in Figure 3. As the result, nine conformers, P5-A1 through P5-A9, were found [point groups: 4 C_{2v}, 4 C_s, and 1 C_1]. Among them, only P5-A9 (C_1 point group) is chiral. Except for the C_1 point group, all of the obtained groups are the subgroups of the C_{4v} point group of the octahedral MXA_5 coordination geometry. The completeness of the enumeration can be confirmed by the orbit-stabilizer theorem as follows. Fixing the X ligand in the positive z direction, 2^5 (= 32) structures of the edge-orienting conformers should be considered. The total number of the structures for each point group is 2 (= 4/2), 4 (= 4/1), and 4 (= 4/1) for the C_{2v}, C_s, and C_1 point groups, respectively, by considering the orders of the rotation groups. Then the total number of considered structures is confirmed to be equal to 32 [2 × 4(for 4 C_{2v}) + 4 × 6(for 4 C_s + 1 C_1 + 1 C_1*) = 32], where the symbol "*" represents the mirror image.

Table 1. Edge-orienting conformers for a $[MX(AB_2)_5]$ complex

Code	Example [a]	Point Group
P5-A1	$[\,[\pm y], [\pm x], [-], [\pm y], [\pm x], [\pm x]\,]$	C_{2v}
P5-A2	$[\,[\pm y], [\pm z], [-], [\pm y], [\pm z], [\pm x]\,]$	C_{2v}
P5-A3	$[\,[\pm z], [\pm x], [-], [\pm z], [\pm x], [\pm x]\,]$	C_{2v}
P5-A4	$[\,[\pm z], [\pm z], [-], [\pm z], [\pm z], [\pm x]\,]$	C_{2v}
P5-A5	$[\,[\pm y], [\pm x], [-], [\pm z], [\pm x], [\pm x]\,]$	C_s
P5-A6	$[\,[\pm y], [\pm z], [-], [\pm z], [\pm z], [\pm x]\,]$	C_s
P5-A7	$[\,[\pm y], [\pm x], [-], [\pm y], [\pm z], [\pm x]\,]$	C_s
P5-A8	$[\,[\pm z], [\pm x], [-], [\pm z], [\pm z], [\pm x]\,]$	C_s
P5-A9 [b]	$[\,[\pm y], [\pm x], [-], [\pm z], [\pm z], [\pm x]\,]$	C_1

[a]Order: (x, y, z, $-x$, $-y$, $-z$). [b]Enantiomeric mirror image exists.

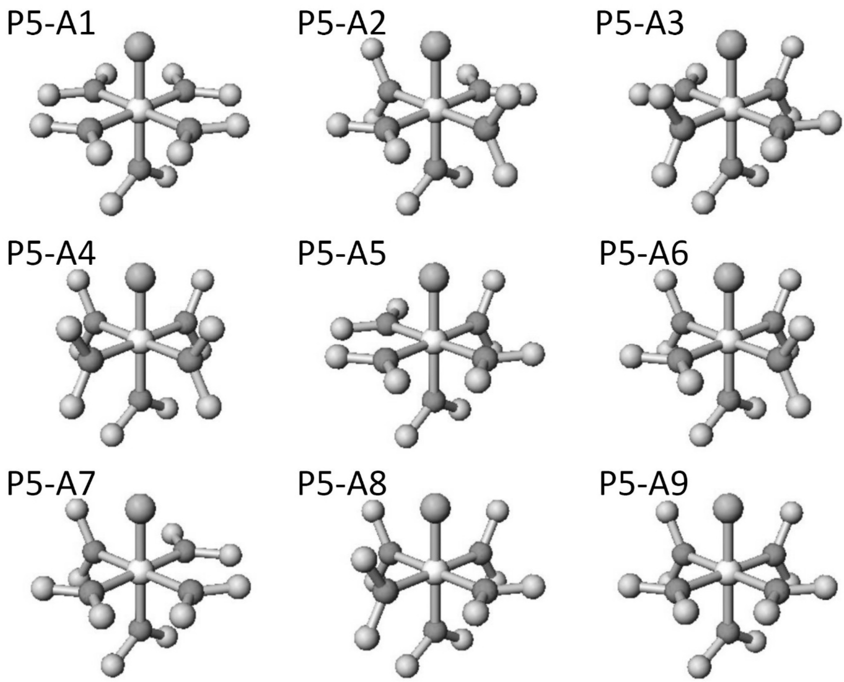

Figure 3. Structures of edge-orienting conformers for $[MX(AB_2)_5]$ complex, P5-A1 – P5-A9.

3.2 Enumeration for octahedral *cis*/*trans*-[$MX_2(AB_2)_4$] complexes

The enumeration was conducted for both the octahedral *cis*- and *trans*-[$MX_2(AB_2)_4$] complexes by the group theory method [29]. The resulting conformers are listed in Tables 2 and 3, and their structures are presented in Figures 4 and 5, respectively. For the *cis*-[$MX_2(AB_2)_4$] complex, seven conformers, P4C-A1 through P4C-A7, were found [2 C_2, 4 C_s, and 1 C_1]. Among them, the C_2 and C_1 conformers are chiral. Except for the C_1 point group, all of the obtained groups are the subgroups of the C_{2v} point group for the octahedral *cis*-MX_2A_4 coordination geometry. The completeness of the enumeration can be confirmed by the orbit-stabilizer theorem as follows. Fixing the two X ligands in the positive x and the positive y directions, 2^4 (= 16) structures of the edge-orienting conformers should be considered. The total number of the structures for each point group is 1 (= 2/2), 2 (= 2/1), and 2 (= 2/1) for the C_2, C_s, and C_1 point groups, respectively, by considering the orders of the rotation groups. Then the total number of considered structures is confirmed to be equal to 16 [1 × 4(for 2 C_2 + 2 C_2*) + 2 × 6(for 4 C_s + 1 C_1 + 1 C_1*) = 16], where the symbol "*" represents the mirror image.

Table 2. Edge-orienting conformers for a *cis*-[$MX_2(AB_2)_4$] complex

Code	Example [a]	Point Group
P4C-A1 [b]	$[\,[-], [-], [\pm x], [\pm z], [\pm z], [\pm y]\,]$	C_2
P4C-A2 [b]	$[\,[-], [-], [\pm x], [\pm y], [\pm x], [\pm y]\,]$	C_2
P4C-A3	$[\,[-], [-], [\pm x], [\pm z], [\pm z], [\pm x]\,]$	C_s
P4C-A4	$[\,[-], [-], [\pm x], [\pm z], [\pm x], [\pm x]\,]$	C_s
P4C-A5	$[\,[-], [-], [\pm x], [\pm y], [\pm z], [\pm x]\,]$	C_s
P4C-A6	$[\,[-], [-], [\pm x], [\pm y], [\pm x], [\pm x]\,]$	C_s
P4C-A7 [b]	$[\,[-], [-], [\pm x], [\pm z], [\pm x], [\pm y]\,]$	C_1

a Order: (x, y, z, $-x$, $-y$, $-z$). *b* Enantiomeric mirror image exists.

For the *trans*-[$MX_2(AB_2)_4$] complex, six conformers, P4T-A1 through P4T-A6, were found [2 D_{4h}, 1 D_{2h}, and 3 C_{2v}]. Among them, none of the conformers are chiral. All of the obtained groups are the subgroups of the D_{4h} point group for the octahedral *trans*-MX_2A_4 coordination geometry. The completeness of the enumeration can be confirmed as follows. Fixing the two X ligands in the positive z and the negative z directions, 2^4 (= 16) structures of the edge-orienting conformers should be considered. The total number of the structures for each point group is 1 (= 8/8), 2 (= 8/4), and 4 (= 8/2) for the D_{4h}, D_{2h}, and C_{2v}. point groups, respectively, by considering the orders of the rotation groups. Then the total number of considered structures is confirmed to be equal to 16 [1 × 2(for 2 D_{4h}) + 2 × 1(for 1 D_{2h}) + 4 × 3(3 C_{2v}) = 16], where the symbol "*" represents the mirror image.

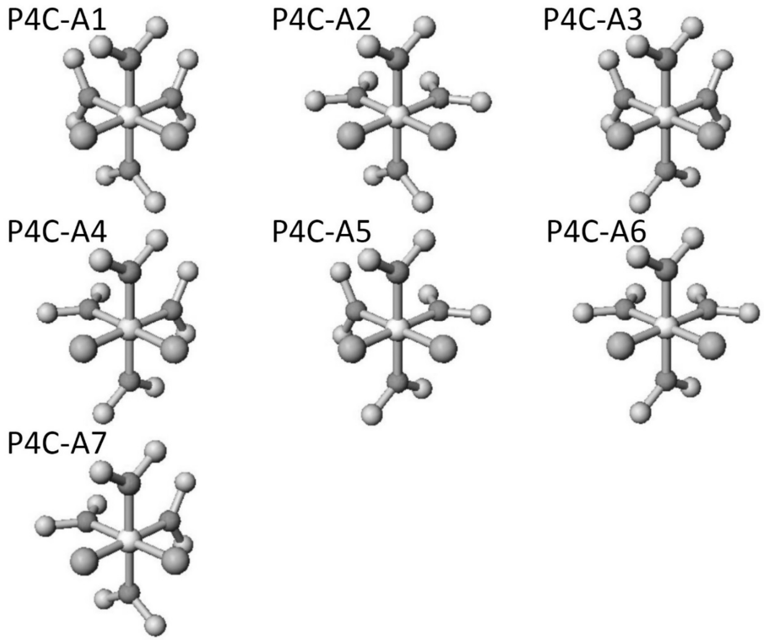

Figure 4. Structures of edge-orienting conformers for *cis*-[$MX_2(AB_2)_4$] complex, P4C-A1 – P4C-A7.

Table 3. Edge-orienting conformers for a *trans*-[$MX_2(AB_2)_4$] complex

Code	Example [a]	Point Group
P4T-A1	[[$\pm y$], [$\pm x$], [$-$], [$\pm y$], [$\pm x$], [$-$]]	D_{4h}
P4T-A2	[[$\pm z$], [$\pm z$], [$-$], [$\pm z$], [$\pm z$], [$-$]]	D_{4h}
P4T-A3	[[$\pm z$], [$\pm x$], [$-$], [$\pm z$], [$\pm x$], [$-$]]	D_{2h}
P4T-A4	[[$\pm z$], [$\pm x$], [$-$], [$\pm y$], [$\pm x$], [$-$]]	C_{2v}
P4T-A5	[[$\pm z$], [$\pm z$], [$-$], [$\pm y$], [$\pm x$], [$-$]]	C_{2v}
P4T- A6	[[$\pm z$], [$\pm z$], [$-$], [$\pm z$], [$\pm x$], [$-$]]	C_{2v}

[a]Order: (x, y, z, $-x$, $-y$, $-z$).

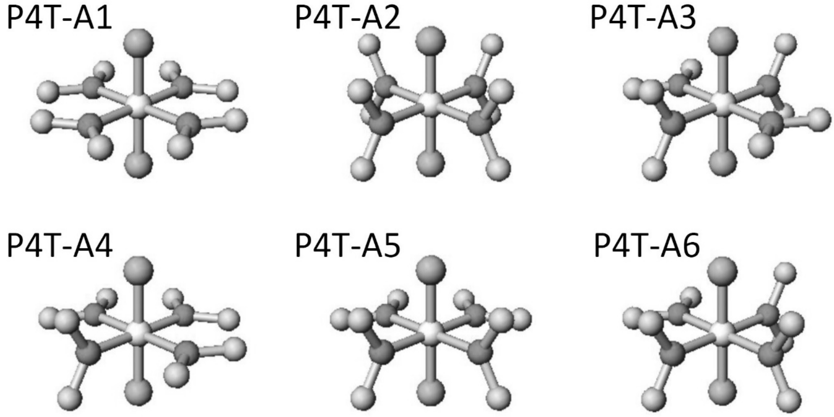

Figure 5. Structures of edge-orienting conformers for *trans*-[$MX_2(AB_2)_4$] complex, P4T-A1 – P4T-A6.

3.3 Enumeration for octahedral *fac*/*mer*-[$MX_3(AB_2)_3$] complexes

The enumeration was conducted for both the octahedral *fac*- and *mer*-[$MX_3(AB_2)_3$] complexes by the group theory method [29]. The resulting conformers are summarized in Tables 4 and 5, and their structures are shown in Figures 6 and 7, respectively. For the *fac*-[$MX_3(AB_2)_3$] complex, two conformers, P3F-A1 and P3F-A2, were obtained. Their point groups are C_3 and C_1, respectively, and both conformers are chiral. Except for the C_1 point group, the obtained group is the subgroup of the C_{3v} point group for the octahedral *fac*-MX_3A_3 coordination geometry. The completeness of the enumeration can be as follows. Fixing the three X ligands in the positive x, positive y, and positive z directions, 2^3 (= 8) structures of the edge-orienting conformers should be considered. The total number of the structures for each point group is 1 (= 3/3) and 3 (= 3/1) for the C_3 and C_1 point groups, respectively, by considering the orders of the rotation groups. Then the total number of considered structures is confirmed to be equal to 8 [1 × 2(for 1 C_3 + 1 C_3*) + 3 × 2(for 1 C_1 + 1 C_1*) = 8], where the symbol "*" represents the mirror image.

Table 4. Edge-orienting conformers for a *fac*-[$MX_3(AB_2)_3$] complex

Code	Example [a]	Point Group
P3F-A1 [b]	[[−], [−], [−], [±z], [±x], [±y]]	C_3
P3F-A2 [b]	[[−], [−], [−], [±z], [±z], [±y]]	C_1

[a]Order: (x, y, z, –x, –y, –z). [b]Enantiomeric mirror image exists.

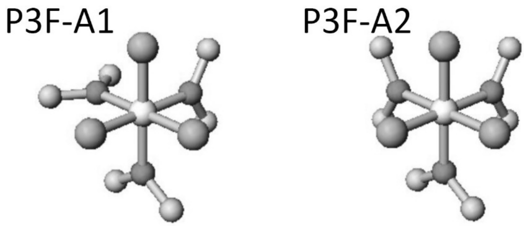

Figure 6. Structures of edge-orienting conformers for *fac*-[$MX_3(AB_2)_3$] complex, P3F-A1 – P3F-A2.

For the *mer*-[$MX_3(AB_2)_3$] complex, six conformers, P3M-A1 through P3M-A6, were obtained [4 C_{2v} and 2 C_s], and none of the conformers are chiral. The obtained group is the subgroup of the C_{2v} point group for the octahedral *mer*-MX_3A_3 coordination geometry. The completeness of the enumeration can be as follows. Fixing the three X ligands in the positive x, positive z, and negative z directions, 2^3 (= 8) structures of the edge-orienting conformers should be considered. The total number of the structures for each point group is 1 (= 2/2) and 2 (= 2/1) for the C_{2v} and C_s point groups, respectively, by considering the orders of the rotation groups. Then the total number of considered structures is confirmed to be equal to 8 [1 × 4(for 4 C_{2v}) + 2 × 2(for 2 C_s) = 8], where the symbol "*" represents the mirror image.

Table 5. Edge-orienting conformers for a *mer*-[$MX_3(AB_2)_3$] complex

Code	Example [a]	Point Group
P3M-A1	[[−], [±x], [−], [±y], [±x], [−]]	C_{2v}
P3M-A2	[[−], [±x], [−], [±z], [±x], [−]]	C_{2v}
P3M-A3	[[−], [±z], [−], [±y], [±z], [−]]	C_{2v}
P3M-A4	[[−], [±z], [−], [±z], [±z], [−]]	C_{2v}
P3M-A5	[[−], [±x], [−], [±y], [±z], [−]]	C_s
P3M-A6	[[−], [±x], [−], [±z], [±z], [−]]	C_s

[a]Order: (x, y, z, –x, –y, –z).

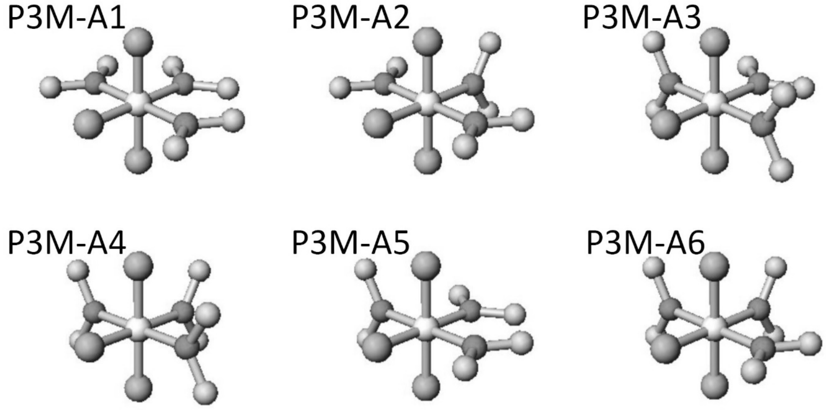

Figure 7. Structures of edge-orienting conformers for *mer*-[$MX_3(AB_2)_3$] complex, P3M-A1–P3M-A6.

3.4 Enumeration for octahedral *cis*/*trans*-[$MX_4(AB_2)_2$] complexes

The enumeration was conducted for both the octahedral *cis*- and *trans*-[$MX_4(AB_2)_2$] complexes by the group theory method [29]. The resulting conformers are listed in Tables 6 and 7, and their structures are presented in Figures 8 and 9, respectively. For the *cis*-[$MX_4(AB_2)_2$] complex, three conformers, P2C-A1 through P2C-A3, were found [2 C_{2v} and 1 C_s], and none of the conformers are chiral. All of the obtained groups are the subgroups of the C_{2v} point group for the octahedral *cis*-MX_4A_2 coordination geometry. The completeness of the enumeration can be confirmed as follows. Fixing the four X ligands in the positive z, the negative x, the negative y, and the negative z directions, 2^2 (= 4) structures of the edge-orienting conformers should be considered. The total number of the structures for each point group is 1 (= 2/2) and 2 (= 2/1) for the C_{2v} and C_s point groups, respectively, by considering the orders of the rotation groups. Then the total number of considered structures is confirmed to be equal to 4 [1 × 2(for 2 C_{2v}) + 2 × 1(for 1 C_s) = 4], where the symbol "*" represents the mirror image.

Table 6. Edge-orienting conformers for a *cis*-[$MX_4(AB_2)_2$] complex

Code	Example ^{a}	Point Group
P2C-A1	[[$\pm y$], [$\pm x$], [$-$], [$-$], [$-$], [$-$]]	C_{2v}
P2C-A2	[[$\pm z$], [$\pm z$], [$-$], [$-$], [$-$], [$-$]]	C_{2v}
P2C-A3	[[$\pm z$], [$\pm x$], [$-$], [$-$], [$-$], [$-$]]	C_s

^{a}Order: (x, y, z, $-x$, $-y$, $-z$).

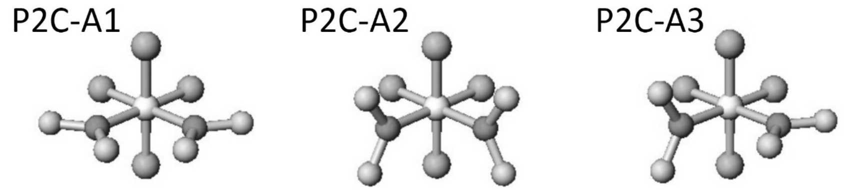

Figure 8. Structures of edge-orienting conformers for *cis*-[$MX_4(AB_2)_2$] complex, P2C-A1 – P2C-A3.

For the *trans*-[$MX_4(AB_2)_2$] complex, two conformers, P2T-A1 and P2T-A2, were found [D_{2h} and D_{2d}], and none of the conformers are chiral. All of the obtained groups are the subgroups of the D_{4h} point group for the octahedral *trans*-MX_4A_2 coordination geometry. The completeness of the enumeration can be confirmed as follows. Fixing the four X ligands in the positive and negative x directions and the positive and negative y directions, 2^2 (= 4) structures of the edge-orienting conformers should be considered. The total number of the structures for each point group is 2 (= 8/4) and 2 (= 8/4) for the D_{2h} and D_{2d}. point groups, respectively, by considering the orders of the rotation groups. Then the total number of considered structures is confirmed to be equal to 4 [2 × 1(for 1 D_{2h}) + 2 × 1(for 1 D_{2d}) = 4], where the symbol "*" represents the mirror image.

Table 7. Edge-orienting conformers for a *trans*-[$MX_4(AB_2)_2$] complex

Code	Example ^{a}	Point Group
P2T-A1	[[$-$], [$-$], [$\pm x$], [$-$], [$-$], [$\pm x$]]	D_{2h}
P2T-A2	[[$-$], [$-$], [$\pm x$], [$-$], [$-$], [$\pm y$]]	D_{2d}

^{a}Order: (x, y, z, $-x$, $-y$, $-z$).

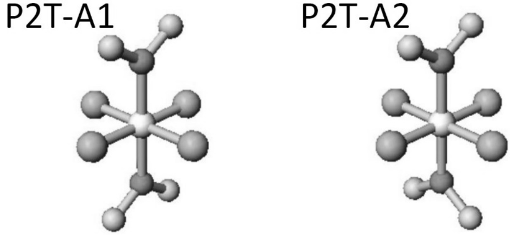

Figure 9. Structures of edge-orienting conformers for *trans*-$[MX_4(AB_2)_2]$ complex, P2T-A1 – P2T-A2.

3.5 Enumeration for octahedral $[MX_5(AB_2)]$ complexes

The enumeration was conducted for the octahedral $[MX_5(AB_2)]$ complex to complete the work of this series. Only one conformer, P1-A1, was found as listed in Table 8 and as depicted in Figure 10. The point group is C_{2v}, which is not chiral, and this point group is the subgroup of the C_{4v} point group of the octahedral MX_5A coordination geometry. The completeness of the enumeration can be confirmed as follows. Fixing the five X ligands in the positive and negative x directions, the positive and negative y directions, and the negative z direction, two edge-orienting structures should be considered. The total number of the structures for the C_{2v} point group is 2 (= 4/2) by considering the orders of the C_{4v} and C_{2v} rotation groups. Then the total number of considered structures is confirmed to be equal to 2 [2 × 1(for 1 C_{2v}) = 2].

Table 8. Edge-orienting conformers for a $[MX_5(AB_2)]$ complex

Code	Example [a]	Point Group
P1-A1	[[−], [−], [$\pm x$], [−], [−], [−]]	C_{2v}

[a]Order: (x, y, z, $-x$, $-y$, $-z$).

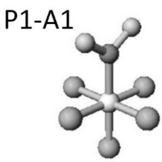

Figure 10. Structures of edge-orienting conformers for $[MX(AB_2)_5]$ complex, P5-A1 – P5-A9.

4 Concluding remarks

In this study, conformers were enumerated on the basis of group theory method for octahedral $[MX_{6-n}(AB_2)_n]$ ($n = 1 - 5$) complexes: $[MX(AB_2)_5]$, *cis*-$[MX_2(AB_2)_4]$, *trans*-$[MX_2(AB_2)_4]$, *fac*-$[MX_3(AB_2)_3]$, *mer*-$[MX_3(AB_2)_3]$, *cis*-$[MX_4(AB_2)_2]$, *trans*-$[MX_4(AB_2)_2]$, and $[MX_5(AB_2)]$ complexes. Using the enumeration result, summarized in Tables 1-8, and the previous result for the $[M(AB_2)_6]$ complex, conformational analysis can be fully conducted for various types of octahedral metal complexes with pyridine ligands. Such research is expected to be useful for the development of metal complexes with valuable functions including catalytic activity.

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