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Enumeration of Edge-Oriented Conformers of Octahedral [M(ABC)$_6$] Complex on the Basis of Computational Group Theory

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Abstract

Edge-oriented conformers of [M(ABC)6] complex have been enumerated on the basis of computational group theory, where M is the central metal, and ABC is the bent triatomic ligand, bound to M through A. Based on the 38 edge-oriented diastereomers of the M(AB)6 core unit, 22835 edge-oriented diastereomers have been found for the [M(ABC)6] complex, which are assigned to seven point groups, 3 D3, 6 S6, 27 C3, 132 C2, 3 Cs, 43 Ci, and 22621 C1.

1 Introduction

Enumeration of the conformers of transition metal complexes is an important issue in conformational analysis, because an increase in the coordination number causes a significant increase of the number of conformers. The conformers of an octahedral [M(AB)$_6$] complex molecule (Figure 1a) have been enumerated [1,2] by the computational group theory (CGT) method [3], where M is the central metal of the molecule, and AB is the diatomic ligand including the donor atom, A. The conformers were first categorized in

two typical orientations of the AB ligand, the edge-direction orientation and the bisecting-direction orientation (Figure 2). For the edge orientation, 38 diastereomers were found, being classified into the following point groups: 1 D_3, 2 C_3, 2 S_6, 4 C_2, 1 C_i, 1 C_s, and 27 C_1. For the bisecting orientation, 16 diastereomers were found and classified into 1 D_{3d}, 1 D_3, 1 S_6, 1 C_{2h}, 5 C_2, 1 C_s, and 6 C_1. This enumeration was found to be useful in the conformational analysis for a nickel(II) complex, $[Ni(nmf)_6]^{2+}$ (hexakis(*N*-methyl formamide-κO)nickel(II) dication), to predict the conformation in a crystal [2].

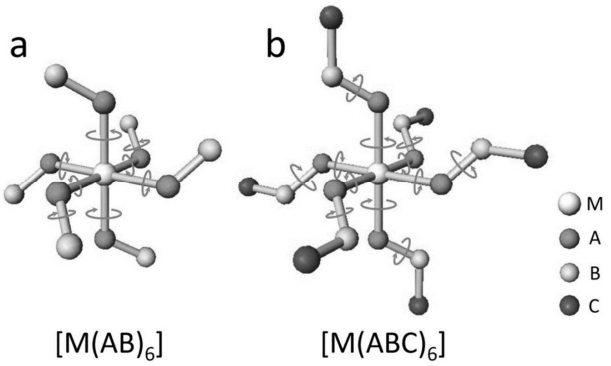

Figure 1. Structures of octahedral metal complexes, $[M(AB)_6]$ (a) and $[M(ABC)_6]$ (b)

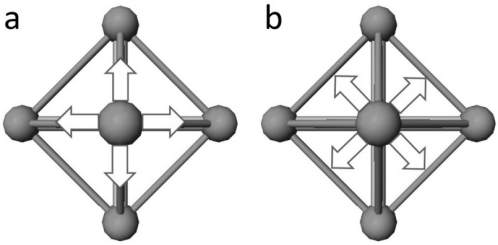

Figure 2. Edge directions (a) and bisecting directions (b) from an apex of an octahedron

In the case of the extended $[M(ABC)_6]$ complex (Figure 1b), the diastereomers have been successfully enumerated only for the bisecting-oriented complex [4], where ABC is a bent triatomic ligand possessing a donor atom, A. The enumerated 7173 conformers were classified into 1 D_{3d}, 4 D_3, 4 S_6, 5 C_{2h}, 7 C_3, 182 C_2, 15 C_s, 23 C_i, and 6932 C_1. The result was really useful not only in predicting the crystal structure of $[Zn(dmso)_6](BPh_4)_2$ [5], but also in considering the molecular motion in crystals and the phase-transition behavior of $[Co(dmso)_6](BPh_4)_2$ [6], where dmso represents dimethylsulfoxide. This success was of course because the compounds had the bisecting-oriented octahedral structure.

On the contrary, however, the enumeration for the edge-oriented $[M(ABC)_6]$ complex (Figure 1b) has not been done, because it is more complicated. Therefore, in this study, enumeration of the conformers was conducted for edge-oriented $[M(ABC)_6]$ complex. The obtained result is expected to be useful in conformational analysis of related metal complexes, including $[Ni(dmso)_6](BPh_4)_2$ [7].

2 Methods

Conformers were obtained based on the computational group theory (CGT) method [3], which was performed using GAP program [8] on Intel Core i7-3770 (3.40GHz) computer. Three-dimensional models were drawn by Winmostar software [9], and the point groups were ascertained by the software.

3 Results and discussion

Conformers of edge-oriented $[M(ABC)_6]$ complex were considered based on the previously enumerated conformers of edge-oriented $[M(AB)_6]$ complex [1,2]. Thirty-eight edge-oriented diastereomers (meridional diastereomers) of $[M(AB)_6]$ complex are listed in Table 1. In this table, for example, a conformer shown in Figure 3 is described as [[y], [-z],

[-y], [z], [-x], [x]] in the order of the numbering system [x, y, z, -x, -y, -z]. In this study, based on the edge-oriented $M(AB)_6$ unit, each ligand, AB, was extended from atom B to atom C to consider the conformers of edge-oriented $[M(ABC)_6]$ complex. For the extension of C, three directions were considered whose dihedral angles M-A-B-C were 180° (anti conformer), 300° (gauche conformer), and 60° (gauche conformer). This is generally sufficient for the purpose of conformational analysis.

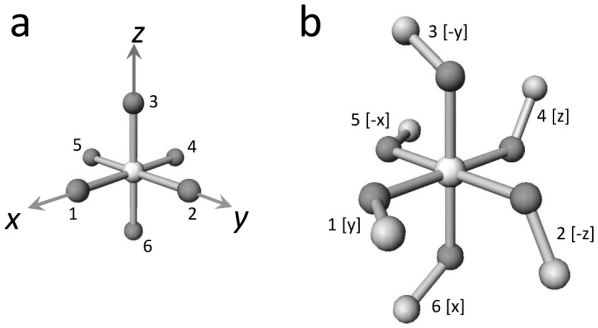

Figure 3. Numbering system (a) and an example of a conformer (b)

Table 1. Edge-oriented conformers of $[M(AB)_6]$ [1]

No	Example	Point Group
A1	[[y], [-z], [-y], [z], [-x], [x]]	D_3
A2	[[y], [z], [-x], [y], [z], [-x]]	C_3
A3	[[y], [-x], [-x], [-z], [-z], [y]]	C_3
A4	[[y], [z], [x], [-y], [-z], [-x]]	S_6
A5	[[y], [-z], [x], [-y], [z], [-x]]	S_6
A6	[[y], [-x], [x], [-z], [-x], [x]]	C_2
A7	[[y], [-z], [y], [z], [-x], [-x]]	C_2
A8	[[y], [-x], [-y], [-y], [-z], [y]]	C_2
A9	[[y], [z], [-y], [-z], [-x], [x]]	C_2
A10	[[y], [-x], [x], [-y], [x], [-x]]	C_i
A11	[[y], [-x], [y], [-z], [-x], [y]]	C_1
A12	[[y], [-x], [-x], [-z], [-x], [y]]	C_1

A13	[[y], [-x], [y], [-z], [z], [y]]	C_1
A14	[[y], [-x], [-x], [-y], [-z], [-x]]	C_1
A15	[[y], [-x], [y], [-y], [-z], [y]]	C_1
A16	[[y], [-x], [-x], [-y], [x], [-x]]	C_s
A17	[[y], [-x], [-y], [z], [-x], [-y]]	C_1
A18	[[y], [-z], [-x], [-y], [-z], [-x]]	C_1
A19	[[y], [-z], [-y], [-y], [-z], [-x]]	C_1
A20	[[y], [-z], [y], [-y], [-z], [-x]]	C_1
A21	[[y], [z], [-x], [-y], [-z], [-x]]	C_1
A22	[[y], [-x], [x], [-z], [-x], [y]]	C_1
A23	[[y], [-x], [-y], [z], [-x], [x]]	C_1
A24	[[y], [-x], [y], [-z], [-x], [x]]	C_1
A25	[[y], [z], [-x], [-z], [z], [-y]]	C_1
A26	[[y], [-z], [-x], [-y], [x], [-x]]	C_1
A27	[[y], [-z], [y], [-z], [-x], [x]]	C_1
A28	[[y], [-x], [-y], [-y], [-z], [-x]]	C_1
A29	[[y], [-z], [-y], [-z], [-x], [x]]	C_1
A30	[[y], [-x], [y], [-y], [-z], [-x]]	C_1
A31	[[y], [-x], [x], [-y], [-z], [-x]]	C_1
A32	[[y], [-x], [-x], [-z], [z], [-y]]	C_1
A33	[[y], [-x], [y], [-y], [z], [-x]]	C_1
A34	[[y], [-z], [y], [-y], [x], [-x]]	C_1
A35	[[y], [-x], [x], [-y], [z], [-x]]	C_1
A36	[[y], [-x], [-y], [-y], [x], [-x]]	C_1
A37	[[y], [-z], [-x], [-y], [x], [-y]]	C_1
A38	[[y], [z], [-x], [-y], [x], [-y]]	C_1

The resulting conformers are summarized in Tables 2, 3, and S1. For example, from conformer A1 of the $M(AB)_6$ unit (D_3 point group), 138 diastereomers of $[M(ABC)_6]$ complex have been derived as listed in Table 2. The 138 diastereomers consist of 3 D_3, 3 C_3, 24 C_2, and 108 C_1 structures. Since all of these diastereomers are chiral, the number of corresponding conformers is 276. Although the 276 conformers have different structures, their $M(AB)_6$ core units have the same structures, belonging to the D_3 point group. Among the A1 related 276 diastereomers, for example, the structures of diastereomers A1-1, A1-2, and A1-3 are shown in Figure 4. The numbering is shown in Table S1, and the three

diastereomers are belonging to the D_3 point group. In A1-1, all the dihedral M-A-B-C angles are 180°. In A1-2 and A1-3, all of the dihedral angles are 60° and 300°, respectively.

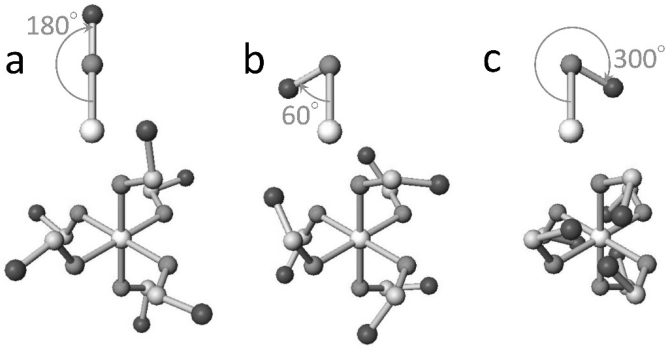

Figure 4. Diastereomers A1-1 (a), A1-2 (b), and A1-3 (c)

In the same way, the rest of the conformers of the [M(ABC)$_6$] complex have been considered based on the M(AB)$_6$ core units from A2 to A38, and the point groups of the obtained diastereomers are also included in Table 2. In total, 45618 conformers, corresponding 22835 diastereomers, have been found as the edge-oriented conformers of [M(ABC)$_6$] complex. In Table 3, the diastereomers and conformers are re-categorized based on the resulting seven-point groups, D_3, S_6, C_3, C_2, C_s, C_i, and C_1. Except for the C_1 symmetry, all of the edge-oriented diastereomers of [M(ABC)$_6$] are tabled in Table S1 in supporting information.

Table 2. Conformers of edge-oriented [M(ABC)$_6$] derived from M(AB)$_6$ core unit

No	Point group of M(AB)$_6$ core unit	Point groups of [M(ABC)$_6$] diastereomer	Total number of diastereomers	Total number of conformers
A1	D_3	3 D_3, 3 C_3, 24 C_2, 108 C_1	138	276
A2	C_3	9 C_3, 240 C_1	249	498
A3	C_3	9 C_3, 240 C_1	249	498
A4	S_6	3 S_6, 3 C_3, 8 C_i, 116 C_1	130	249
A5	S_6	3 S_6, 3 C_3, 8 C_i, 116 C_1	130	249

A6	C_2	27 C_2, 351 C_1	378	756
A7	C_2	27 C_2, 351 C_1	378	756
A8	C_2	27 C_2, 351 C_1	378	756
A9	C_2	27 C_2, 351 C_1	378	756
A10	C_i	27 C_i, 351 C_1	378	729
A11	C_1	729 C_1	729	1458
A12	C_1	729 C_1	729	1458
A13	C_1	729 C_1	729	1458
A14	C_1	729 C_1	729	1458
A15	C_1	729 C_1	729	1458
A16	C_s	3 C_s, 363 C_1	366	729
A17	C_1	729 C_1	729	1458
A18	C_1	729 C_1	729	1458
A19	C_1	729 C_1	729	1458
A20	C_1	729 C_1	729	1458
A21	C_1	729 C_1	729	1458
A22	C_1	729 C_1	729	1458
A23	C_1	729 C_1	729	1458
A24	C_1	729 C_1	729	1458
A25	C_1	729 C_1	729	1458
A26	C_1	729 C_1	729	1458
A27	C_1	729 C_1	729	1458
A28	C_1	729 C_1	729	1458
A29	C_1	729 C_1	729	1458
A30	C_1	729 C_1	729	1458
A31	C_1	729 C_1	729	1458
A32	C_1	729 C_1	729	1458
A33	C_1	729 C_1	729	1458
A34	C_1	729 C_1	729	1458
A35	C_1	729 C_1	729	1458
A36	C_1	729 C_1	729	1458
A37	C_1	729 C_1	729	1458
A38	C_1	729 C_1	729	1458
		Total	22835	45618

Table 3. Conformers of edge-oriented $[M(ABC)_6]$

No	Point group of $[M(ABC)_6]$ conformer	Total number of diastereomers	Total number of conformers
1	D_3	3	6
2	S_6	6	6
3	C_3	27	54
4	C_2	132	264
5	C_s	3	3
6	C_i	43	43
7	C_1	22621	45242
	Total	22835	45618

In the crystal of the nickel(II) complex, $[Ni(dmso)_6](BPh_4)_2$, two crystallographically distinguished $[Ni(dmso)_6]^{2+}$ cations were included [7], and one had the bisecting-oriented octahedral structure and the other had the edge-oriented structure (Figure 5a). From the

result of enumeration in this study, the edge-oriented structure is assigned to diastereomer A4-3 (S_6 point group) in Table S1, where M-A-B-C corresponds to Ni-O-S-Lp (Lp: lone pair).

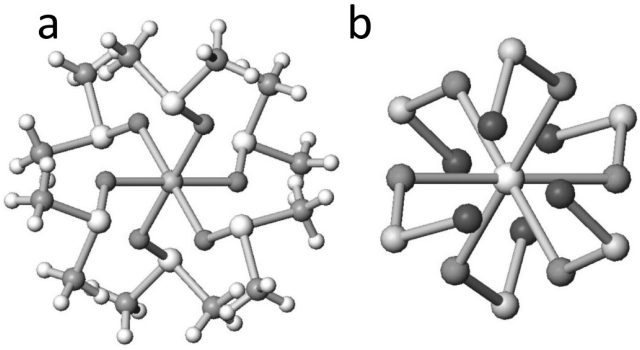

Figure 5. Edge-oriented $[Ni(dmso)_6]^{2+}$ cation (a) and diastereomer A4-3 (b)

4 Concluding remarks

In this study, edge-oriented conformers of octahedral $[M(ABC)_6]$ complex have been enumerated on the basis of computational group theory. Based on the 38 edge-oriented diastereomers of the $M(AB)_6$ core unit, 22835 diastereomers, corresponding 45618 conformers, have been found for the $[M(ABC)_6]$ complex, considering the anti and gauche conformations. The obtained diastereomers are assigned to seven point groups, 3 D_3, 6 S_6, 27 C_3, 132 C_2, 3 C_s, 43 C_i, and 22621 C_1. The results are summarized in tables, which is useful in conformational analysis of the related octahedral complexes.

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Supporting Information: Table S1.

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Supporting information

Table S1. Diasterepmers except for C_1 (the structures of the cenrtal $M(AB)_6$ units are shown in their abbreviation forms; the numbers 0, 1, and 2 correspond to the dihedral angles of M-A-B-C 180°, 300°, and 60°, respectively)

No.	Diastereomer	Point group
-A1-		
A1-1	| y|-z|-y| z|-x| x|:[0, 0, 0, 0, 0, 0]	D_3
A1-2	| y|-z|-y| z|-x| x|:[2, 2, 2, 2, 2, 2]	D_3
A1-3	| y|-z|-y| z|-x| x|:[1, 1, 1, 1, 1, 1]	D_3
A1-4	| y|-z|-y| z|-x| x|:[2, 2, 0, 0, 0, 2]	C_3
A1-5	| y|-z|-y| z|-x| x|:[1, 1, 0, 0, 0, 1]	C_3
A1-6	| y|-z|-y| z|-x| x|:[2, 2, 1, 1, 1, 2]	C_3
A1-7	| y|-z|-y| z|-x| x|:[1, 2, 1, 0, 2, 0]	C_2
A1-8	| y|-z|-y| z|-x| x|:[0, 2, 0, 0, 2, 0]	C_2
A1-9	| y|-z|-y| z|-x| x|:[2, 2, 2, 0, 2, 0]	C_2
A1-10	| y|-z|-y| z|-x| x|:[0, 2, 2, 0, 1, 1]	C_2
A1-11	| y|-z|-y| z|-x| x|:[0, 2, 2, 0, 2, 2]	C_2
A1-12	| y|-z|-y| z|-x| x|:[0, 2, 2, 0, 0, 0]	C_2
A1-13	| y|-z|-y| z|-x| x|:[1, 0, 1, 0, 1, 1]	C_2
A1-14	| y|-z|-y| z|-x| x|:[1, 0, 1, 0, 0, 0]	C_2
A1-15	| y|-z|-y| z|-x| x|:[2, 0, 1, 0, 2, 1]	C_2
A1-16	| y|-z|-y| z|-x| x|:[0, 0, 1, 0, 0, 1]	C_2
A1-17	| y|-z|-y| z|-x| x|:[1, 1, 1, 0, 1, 0]	C_2
A1-18	| y|-z|-y| z|-x| x|:[0, 1, 1, 0, 1, 1]	C_2
A1-19	| y|-z|-y| z|-x| x|:[0, 1, 1, 0, 2, 2]	C_2
A1-20	| y|-z|-y| z|-x| x|:[0, 1, 1, 0, 0, 0]	C_2
A1-21	| y|-z|-y| z|-x| x|:[0, 0, 0, 0, 2, 2]	C_2
A1-22	| y|-z|-y| z|-x| x|:[1, 0, 2, 0, 1, 2]	C_2
A1-23	| y|-z|-y| z|-x| x|:[2, 0, 2, 0, 2, 2]	C_2
A1-24	| y|-z|-y| z|-x| x|:[2, 1, 2, 0, 1, 0]	C_2
A1-25	| y|-z|-y| z|-x| x|:[1, 2, 1, 2, 1, 1]	C_2
A1-26	| y|-z|-y| z|-x| x|:[1, 2, 1, 2, 2, 2]	C_2
A1-27	| y|-z|-y| z|-x| x|:[2, 2, 1, 2, 2, 1]	C_2
A1-28	| y|-z|-y| z|-x| x|:[1, 2, 2, 2, 1, 2]	C_2
A1-29	| y|-z|-y| z|-x| x|:[1, 2, 1, 1, 2, 1]	C_2
A1-30	| y|-z|-y| z|-x| x|:[1, 2, 2, 1, 1, 1]	C_2
-A2-		
A2-1	| y| z|-x| y| z|-x|:[2, 0, 0, 0, 2, 2]	C_3
A2-2	| y| z|-x| y| z|-x|:[0, 2, 2, 2, 0, 0]	C_3
A2-3	| y| z|-x| y| z|-x|:[0, 0, 0, 0, 0, 0]	C_3
A2-4	| y| z|-x| y| z|-x|:[0, 1, 1, 1, 0, 0]	C_3
A2-5	| y| z|-x| y| z|-x|:[1, 0, 0, 0, 1, 1]	C_3
A2-6	| y| z|-x| y| z|-x|:[1, 2, 2, 2, 1, 1]	C_3
A2-7	| y| z|-x| y| z|-x|:[1, 1, 1, 1, 1, 1]	C_3
A2-8	| y| z|-x| y| z|-x|:[2, 2, 2, 2, 2, 2]	C_3
A2-9	| y| z|-x| y| z|-x|:[2, 1, 1, 1, 2, 2]	C_3
-A3-		
A3-1	| y|-x|-x|-z|-z| y|:[1, 0, 1, 0, 1, 0]	C_3
A3-2	| y|-x|-x|-z|-z| y|:[0, 2, 0, 2, 0, 2]	C_3

A3-3	| y|-x|-x|-z|-z| y|:[0, 0, 0, 0, 0, 0]	C_3
A3-4	| y|-x|-x|-z|-z| y|:[0, 1, 0, 1, 0, 1]	C_3
A3-5	| y|-x|-x|-z|-z| y|:[2, 0, 2, 0, 2, 0]	C_3
A3-6	| y|-x|-x|-z|-z| y|:[1, 2, 1, 2, 1, 2]	C_3
A3-7	| y|-x|-x|-z|-z| y|:[2, 2, 2, 2, 2, 2]	C_3
A3-8	| y|-x|-x|-z|-z| y|:[1, 1, 1, 1, 1, 1]	C_3
A3-9	| y|-x|-x|-z|-z| y|:[2, 1, 2, 1, 2, 1]	C_3

-A4----------

A4-1	| y| z| x|-y|-z|-x|:[0, 0, 0, 0, 0, 0]	S_6
A4-2	| y| z| x|-y|-z|-x|:[1, 1, 1, 2, 2, 2]	S_6
A4-3	| y| z| x|-y|-z|-x|:[2, 2, 2, 1, 1, 1]	S_6
A4-4	| y| z| x|-y|-z|-x|:[1, 1, 1, 0, 0, 0]	C_3
A4-5	| y| z| x|-y|-z|-x|:[2, 2, 2, 0, 0, 0]	C_3
A4-6	| y| z| x|-y|-z|-x|:[1, 1, 1, 1, 1, 1]	C_3
A4-7	| y| z| x|-y|-z|-x|:[0, 1, 2, 0, 2, 1]	C_i
A4-8	| y| z| x|-y|-z|-x|:[0, 1, 1, 0, 2, 2]	C_i
A4-9	| y| z| x|-y|-z|-x|:[0, 1, 0, 0, 2, 0]	C_i
A4-10	| y| z| x|-y|-z|-x|:[0, 2, 2, 0, 1, 1]	C_i
A4-11	| y| z| x|-y|-z|-x|:[0, 2, 1, 0, 1, 2]	C_i
A4-12	| y| z| x|-y|-z|-x|:[0, 2, 0, 0, 1, 0]	C_i
A4-13	| y| z| x|-y|-z|-x|:[2, 1, 2, 1, 2, 1]	C_i
A4-14	| y| z| x|-y|-z|-x|:[2, 1, 1, 1, 2, 2]	C_i

-A5----------

A5-1	| y|-z| x|-y| z|-x|:[0, 0, 0, 0, 0, 0]	S_6
A5-2	| y|-z| x|-y| z|-x|:[1, 2, 2, 2, 1, 1]	S_6
A5-3	| y|-z| x|-y| z|-x|:[2, 1, 1, 1, 2, 2]	S_6
A5-4	| y|-z| x|-y| z|-x|:[2, 0, 0, 0, 2, 2]	C_3
A5-5	| y|-z| x|-y| z|-x|:[0, 2, 2, 2, 0, 0]	C_3
A5-6	| y|-z| x|-y| z|-x|:[1, 1, 1, 1, 1, 1]	C_3
A5-7	| y|-z| x|-y| z|-x|:[1, 0, 2, 2, 0, 1]	C_i
A5-8	| y|-z| x|-y| z|-x|:[2, 0, 2, 1, 0, 1]	C_i
A5-9	| y|-z| x|-y| z|-x|:[0, 0, 2, 0, 0, 1]	C_i
A5-10	| y|-z| x|-y| z|-x|:[0, 1, 2, 0, 2, 1]	C_i
A5-11	| y|-z| x|-y| z|-x|:[0, 1, 1, 0, 2, 2]	C_i
A5-12	| y|-z| x|-y| z|-x|:[0, 1, 0, 0, 2, 0]	C_i
A5-13	| y|-z| x|-y| z|-x|:[2, 2, 2, 1, 1, 1]	C_i
A5-14	| y|-z| x|-y| z|-x|:[2, 1, 2, 1, 2, 1]	C_i

-A6----------

A6-1	| y|-x| x|-z|-x| x|:[1, 0, 2, 1, 2, 0]	C_2
A6-2	| y|-x| x|-z|-x| x|:[2, 2, 0, 2, 0, 2]	C_2
A6-3	| y|-x| x|-z|-x| x|:[0, 0, 2, 0, 2, 0]	C_2
A6-4	| y|-x| x|-z|-x| x|:[0, 2, 0, 0, 0, 2]	C_2
A6-5	| y|-x| x|-z|-x| x|:[2, 0, 2, 2, 2, 0]	C_2
A6-6	| y|-x| x|-z|-x| x|:[1, 2, 0, 1, 0, 2]	C_2
A6-7	| y|-x| x|-z|-x| x|:[2, 0, 0, 2, 0, 0]	C_2
A6-8	| y|-x| x|-z|-x| x|:[1, 0, 0, 1, 0, 0]	C_2
A6-9	| y|-x| x|-z|-x| x|:[2, 1, 0, 2, 0, 1]	C_2
A6-10	| y|-x| x|-z|-x| x|:[1, 0, 1, 1, 1, 0]	C_2
A6-11	| y|-x| x|-z|-x| x|:[0, 0, 0, 0, 0, 0]	C_2
A6-12	| y|-x| x|-z|-x| x|:[0, 1, 0, 0, 0, 1]	C_2
A6-13	| y|-x| x|-z|-x| x|:[0, 0, 1, 0, 1, 0]	C_2
A6-14	| y|-x| x|-z|-x| x|:[1, 1, 0, 1, 0, 1]	C_2
A6-15	| y|-x| x|-z|-x| x|:[2, 0, 1, 2, 1, 0]	C_2
A6-16	| y|-x| x|-z|-x| x|:[0, 2, 1, 0, 1, 2]	C_2

A6-17	| y|-x| x|-z|-x| x|:[0, 1, 1, 0, 1, 1]	C_2
A6-18	| y|-x| x|-z|-x| x|:[0, 2, 2, 0, 2, 2]	C_2
A6-19	| y|-x| x|-z|-x| x|:[0, 1, 2, 0, 2, 1]	C_2
A6-20	| y|-x| x|-z|-x| x|:[2, 2, 1, 2, 1, 2]	C_2
A6-21	| y|-x| x|-z|-x| x|:[1, 1, 2, 1, 2, 1]	C_2
A6-22	| y|-x| x|-z|-x| x|:[1, 2, 1, 1, 1, 2]	C_2
A6-23	| y|-x| x|-z|-x| x|:[2, 1, 2, 2, 2, 1]	C_2
A6-24	| y|-x| x|-z|-x| x|:[2, 1, 1, 2, 1, 1]	C_2
A6-25	| y|-x| x|-z|-x| x|:[1, 2, 2, 1, 2, 2]	C_2
A6-26	| y|-x| x|-z|-x| x|:[2, 2, 2, 2, 2, 2]	C_2
A6-27	| y|-x| x|-z|-x| x|:[1, 1, 1, 1, 1, 1]	C_2

-A7----------

A7-1	| y|-z| y| z|-x|-x|:[0, 1, 1, 1, 0, 1]	C_2
A7-2	| y|-z| y| z|-x|-x|:[0, 0, 1, 0, 0, 1]	C_2
A7-3	| y|-z| y| z|-x|-x|:[2, 1, 0, 1, 2, 0]	C_2
A7-4	| y|-z| y| z|-x|-x|:[2, 2, 0, 2, 2, 0]	C_2
A7-5	| y|-z| y| z|-x|-x|:[2, 0, 0, 0, 2, 0]	C_2
A7-6	| y|-z| y| z|-x|-x|:[0, 2, 1, 2, 0, 1]	C_2
A7-7	| y|-z| y| z|-x|-x|:[1, 1, 0, 1, 1, 0]	C_2
A7-8	| y|-z| y| z|-x|-x|:[1, 2, 0, 2, 1, 0]	C_2
A7-9	| y|-z| y| z|-x|-x|:[1, 0, 0, 0, 1, 0]	C_2
A7-10	| y|-z| y| z|-x|-x|:[0, 1, 0, 1, 0, 0]	C_2
A7-11	| y|-z| y| z|-x|-x|:[1, 0, 2, 0, 1, 2]	C_2
A7-12	| y|-z| y| z|-x|-x|:[2, 0, 2, 0, 2, 2]	C_2
A7-13	| y|-z| y| z|-x|-x|:[0, 0, 2, 0, 0, 2]	C_2
A7-14	| y|-z| y| z|-x|-x|:[0, 1, 2, 1, 0, 2]	C_2
A7-15	| y|-z| y| z|-x|-x|:[0, 2, 0, 2, 0, 0]	C_2
A7-16	| y|-z| y| z|-x|-x|:[0, 0, 0, 0, 0, 0]	C_2
A7-17	| y|-z| y| z|-x|-x|:[1, 0, 1, 0, 1, 1]	C_2
A7-18	| y|-z| y| z|-x|-x|:[2, 0, 1, 0, 2, 1]	C_2
A7-19	| y|-z| y| z|-x|-x|:[0, 2, 2, 2, 0, 2]	C_2
A7-20	| y|-z| y| z|-x|-x|:[2, 1, 1, 1, 2, 1]	C_2
A7-21	| y|-z| y| z|-x|-x|:[2, 2, 1, 2, 2, 1]	C_2
A7-22	| y|-z| y| z|-x|-x|:[1, 2, 2, 2, 1, 2]	C_2
A7-23	| y|-z| y| z|-x|-x|:[2, 2, 2, 2, 2, 2]	C_2
A7-24	| y|-z| y| z|-x|-x|:[1, 2, 1, 2, 1, 1]	C_2
A7-25	| y|-z| y| z|-x|-x|:[1, 1, 1, 1, 1, 1]	C_2
A7-26	| y|-z| y| z|-x|-x|:[2, 1, 2, 1, 2, 2]	C_2
A7-27	| y|-z| y| z|-x|-x|:[1, 1, 2, 1, 1, 2]	C_2

-A8----------

A8-1	| y|-x|-y|-y|-z| y|:[1, 1, 1, 0, 1, 0]	C_2
A8-2	| y|-x|-y|-y|-z| y|:[0, 2, 0, 2, 2, 2]	C_2
A8-3	| y|-x|-y|-y|-z| y|:[1, 0, 1, 0, 0, 0]	C_2
A8-4	| y|-x|-y|-y|-z| y|:[0, 0, 0, 2, 0, 2]	C_2
A8-5	| y|-x|-y|-y|-z| y|:[1, 2, 1, 0, 2, 0]	C_2
A8-6	| y|-x|-y|-y|-z| y|:[0, 1, 0, 2, 1, 2]	C_2
A8-7	| y|-x|-y|-y|-z| y|:[0, 2, 0, 0, 2, 0]	C_2
A8-8	| y|-x|-y|-y|-z| y|:[0, 2, 0, 1, 2, 1]	C_2
A8-9	| y|-x|-y|-y|-z| y|:[0, 1, 0, 0, 1, 0]	C_2
A8-10	| y|-x|-y|-y|-z| y|:[2, 1, 2, 0, 1, 0]	C_2
A8-11	| y|-x|-y|-y|-z| y|:[0, 0, 0, 0, 0, 0]	C_2
A8-12	| y|-x|-y|-y|-z| y|:[0, 0, 0, 1, 0, 1]	C_2
A8-13	| y|-x|-y|-y|-z| y|:[2, 0, 2, 0, 0, 0]	C_2
A8-14	| y|-x|-y|-y|-z| y|:[0, 1, 0, 1, 1, 1]	C_2
A8-15	| y|-x|-y|-y|-z| y|:[2, 2, 2, 0, 2, 0]	C_2

A8-16	| y|-x|-y|-y|-z| y|:[2, 0, 2, 2, 0, 2]	C_2
A8-17	| y|-x|-y|-y|-z| y|:[2, 0, 2, 1, 0, 1]	C_2
A8-18	| y|-x|-y|-y|-z| y|:[1, 0, 1, 2, 0, 2]	C_2
A8-19	| y|-x|-y|-y|-z| y|:[1, 0, 1, 1, 0, 1]	C_2
A8-20	| y|-x|-y|-y|-z| y|:[1, 1, 1, 2, 1, 2]	C_2
A8-21	| y|-x|-y|-y|-z| y|:[1, 2, 1, 2, 2, 2]	C_2
A8-22	| y|-x|-y|-y|-z| y|:[2, 2, 2, 2, 2, 2]	C_2
A8-23	| y|-x|-y|-y|-z| y|:[1, 1, 1, 1, 1, 1]	C_2
A8-24	| y|-x|-y|-y|-z| y|:[2, 1, 2, 2, 1, 2]	C_2
A8-25	| y|-x|-y|-y|-z| y|:[1, 2, 1, 1, 2, 1]	C_2
A8-26	| y|-x|-y|-y|-z| y|:[2, 2, 2, 1, 2, 1]	C_2
A8-27	| y|-x|-y|-y|-z| y|:[2, 1, 2, 1, 1, 1]	C_2

-A9----------

A9-1	| y| z|-y|-z|-x| x|:[0, 2, 2, 2, 0, 2]	C_2
A9-2	| y| z|-y|-z|-x| x|:[0, 0, 2, 0, 0, 2]	C_2
A9-3	| y| z|-y|-z|-x| x|:[2, 1, 0, 1, 2, 0]	C_2
A9-4	| y| z|-y|-z|-x| x|:[2, 2, 0, 2, 2, 0]	C_2
A9-5	| y| z|-y|-z|-x| x|:[2, 0, 0, 0, 2, 0]	C_2
A9-6	| y| z|-y|-z|-x| x|:[0, 1, 2, 1, 0, 2]	C_2
A9-7	| y| z|-y|-z|-x| x|:[2, 0, 1, 0, 2, 1]	C_2
A9-8	| y| z|-y|-z|-x| x|:[1, 0, 1, 0, 1, 1]	C_2
A9-9	| y| z|-y|-z|-x| x|:[0, 0, 1, 0, 0, 1]	C_2
A9-10	| y| z|-y|-z|-x| x|:[0, 2, 0, 2, 0, 0]	C_2
A9-11	| y| z|-y|-z|-x| x|:[1, 1, 0, 1, 1, 0]	C_2
A9-12	| y| z|-y|-z|-x| x|:[1, 2, 0, 2, 1, 0]	C_2
A9-13	| y| z|-y|-z|-x| x|:[1, 0, 0, 0, 1, 0]	C_2
A9-14	| y| z|-y|-z|-x| x|:[0, 2, 1, 2, 0, 1]	C_2
A9-15	| y| z|-y|-z|-x| x|:[0, 0, 0, 0, 0, 0]	C_2
A9-16	| y| z|-y|-z|-x| x|:[0, 1, 0, 1, 0, 0]	C_2
A9-17	| y| z|-y|-z|-x| x|:[2, 0, 2, 0, 2, 2]	C_2
A9-18	| y| z|-y|-z|-x| x|:[1, 0, 2, 0, 1, 2]	C_2
A9-19	| y| z|-y|-z|-x| x|:[0, 1, 1, 1, 0, 1]	C_2
A9-20	| y| z|-y|-z|-x| x|:[2, 1, 1, 1, 2, 1]	C_2
A9-21	| y| z|-y|-z|-x| x|:[1, 1, 1, 1, 1, 1]	C_2
A9-22	| y| z|-y|-z|-x| x|:[2, 2, 2, 2, 2, 2]	C_2
A9-23	| y| z|-y|-z|-x| x|:[2, 1, 2, 1, 2, 2]	C_2
A9-24	| y| z|-y|-z|-x| x|:[1, 1, 2, 1, 1, 2]	C_2
A9-25	| y| z|-y|-z|-x| x|:[1, 2, 2, 2, 1, 2]	C_2
A9-26	| y| z|-y|-z|-x| x|:[2, 2, 1, 2, 2, 1]	C_2
A9-27	| y| z|-y|-z|-x| x|:[1, 2, 1, 2, 1, 1]	C_2

-A10----------

A10-1	| y|-x| x|-y| x|-x|:[2, 1, 0, 1, 2, 0]	C_i
A10-2	| y|-x| x|-y| x|-x|:[1, 1, 0, 2, 2, 0]	C_i
A10-3	| y|-x| x|-y| x|-x|:[0, 1, 0, 0, 2, 0]	C_i
A10-4	| y|-x| x|-y| x|-x|:[2, 0, 1, 1, 0, 2]	C_i
A10-5	| y|-x| x|-y| x|-x|:[1, 0, 1, 2, 0, 2]	C_i
A10-6	| y|-x| x|-y| x|-x|:[0, 0, 1, 0, 0, 2]	C_i
A10-7	| y|-x| x|-y| x|-x|:[1, 2, 0, 2, 1, 0]	C_i
A10-8	| y|-x| x|-y| x|-x|:[2, 2, 0, 1, 1, 0]	C_i
A10-9	| y|-x| x|-y| x|-x|:[0, 2, 0, 0, 1, 0]	C_i
A10-10	| y|-x| x|-y| x|-x|:[1, 0, 2, 2, 0, 1]	C_i
A10-11	| y|-x| x|-y| x|-x|:[2, 0, 2, 1, 0, 1]	C_i
A10-12	| y|-x| x|-y| x|-x|:[0, 0, 2, 0, 0, 1]	C_i
A10-13	| y|-x| x|-y| x|-x|:[1, 0, 0, 2, 0, 0]	C_i
A10-14	| y|-x| x|-y| x|-x|:[2, 0, 0, 1, 0, 0]	C_i

A10-15	| y|-x| x|-y| x|-x|:[0, 0, 0, 0, 0, 0]	C_i
A10-16	| y|-x| x|-y| x|-x|:[0, 1, 2, 0, 2, 1]	C_i
A10-17	| y|-x| x|-y| x|-x|:[0, 2, 2, 0, 1, 1]	C_i
A10-18	| y|-x| x|-y| x|-x|:[0, 1, 1, 0, 2, 2]	C_i
A10-19	| y|-x| x|-y| x|-x|:[0, 2, 1, 0, 1, 2]	C_i
A10-20	| y|-x| x|-y| x|-x|:[2, 1, 1, 1, 2, 2]	C_i
A10-21	| y|-x| x|-y| x|-x|:[1, 1, 1, 2, 2, 2]	C_i
A10-22	| y|-x| x|-y| x|-x|:[1, 2, 2, 2, 1, 1]	C_i
A10-23	| y|-x| x|-y| x|-x|:[2, 2, 2, 1, 1, 1]	C_i
A10-24	| y|-x| x|-y| x|-x|:[1, 1, 2, 2, 2, 1]	C_i
A10-25	| y|-x| x|-y| x|-x|:[2, 1, 2, 1, 2, 1]	C_i
A10-26	| y|-x| x|-y| x|-x|:[1, 2, 1, 2, 1, 2]	C_i
A10-27	| y|-x| x|-y| x|-x|:[2, 2, 1, 1, 1, 2]	C_i

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A16-1	| y|-x|-x|-y| x|-x|:[0, 0, 1, 0, 0, 2]	C_s
A16-2	| y|-x|-x|-y| x|-x|:[0, 0, 2, 0, 0, 1]	C_s
A16-3	| y|-x|-x|-y| x|-x|:[0, 0, 0, 0, 0, 0]	C_s
