Journal of Organometallic Chemistry
Elsevier Sequoia S.A., Lausanne
Printed in The Netherlands

ORGANOMETALLIC COMPOUNDS XVIII*. TOPOLOGICAL REPRESENTATION OF INTRAMOLECULAR ISOMERIZATION REACTIONS OF OCTAHEDRAL COMPLEXES VIA TRIGONAL OR RHOMBIC TWISTS

M. GIELEN AND J. TOPART**
Université Libre de Bruxelles, Faculté des Sciences, Service de Chimie Organique, 50, avenue F. D. Roosevelt, Bruxelles 5 (Belgium)

(Received March 26th, 1969)

SUMMARY

Topological and matrix representations are given for the intramolecular isomerization reactions of six-coordinate complexes via trigonal or rhombic twists.

INTRODUCTION

Topological representations have already been given for the intramolecular isomerizations of some simple octahedral complexes[2]. The number of dimensions which must be used for this description depends on the complexity of the chemical system. Nevertheless, a matrix representation, which is readily generated from the general case[1], may sometimes be the only recourse if the class cannot be described in a projection of a three-dimensional, non interpenetrating figure[3,4]. Topological illustrations are desirable in two and three-dimensional representations because all pathways and the degeneracies[3] of the different subgroups are immediately apparent. We therefore wish to introduce a series of representations for more complex systems which have not yet been described.

RESULTS

123,455 *systems****

It is possible to transform the 30 by 30 reaction matrix $R(123,456)$*** into a 15 by 15$R(123,455)$ matrix[1], which may be converted into a topological description[2], the non-zero elements being the turning-points (or transition states) to go from one isomer to another. It consists of a hexagonal prism (see Fig. 1), the six parallel edges of which representing the degenerate paths ($r_{ki}=2$). The three inactive isomers (h, g

* Fort Part XVII see ref. 1.
** Titulaire d'une bourse de specialisation de l'I.R.S.I.A.
*** For the numbering convention and symbolism see ref. 2; a=123,456; b=123,645; c=123,564; d=125,463; e=126,435; f=136,425; g=125,643; h=126,534; i=135,426; j=124,653; k=135,624; l=125,436; m=125,346; n=123,654 and q=123,465.

and k) are to be placed each in one of the three diagonal planes of this prism and are to be connected with all the points of the figure except those lying in this plane.

$R(123,455) =$

	a	$\bar{b}$	c	$\bar{d}$	e	f	g	h	k	$\bar{a}$	b	$\bar{c}$	$\bar{d}$	$\bar{e}$	$\bar{f}$
a	0	0	1	0	1	2	1	1	0	0	1	0	1	0	0
$\bar{b}$	0	0	0	0	0	1	0	1	1	1	0	1	2	1	0
c	1	0	0	0	0	0	1	0	1	0	1	0	1	2	1
$\bar{d}$	0	0	0	0	0	1	0	1	1	1	2	1	0	1	0
e	1	0	0	0	0	0	1	0	1	0	1	2	1	0	1
f	2	1	0	1	0	0	1	1	0	0	0	1	0	1	0
g	1	0	1	0	1	1	0	0	0	1	0	1	0	1	1
h	1	1	0	1	0	1	0	0	0	1	1	0	1	0	1
k	0	1	1	1	1	0	0	0	0	1	1	1	0	1	0
$\bar{a}$	0	1	0	1	0	0	1	1	0	0	0	1	0	1	2
b	1	0	1	2	1	0	0	1	1	0	0	0	0	0	1
$\bar{c}$	0	1	0	1	2	1	1	0	1	1	0	0	0	0	0
d	1	2	1	0	1	0	0	1	1	0	0	0	0	0	1
$\bar{e}$	0	1	2	1	0	1	1	0	1	1	0	0	0	0	0
$\bar{f}$	0	0	1	0	1	0	1	1	0	0	1	0	0	0	0

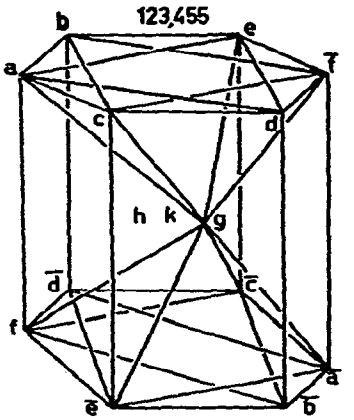

Fig. 1. Topological representation of the isomerization reactions of 123,455.

$R(123,455)$ may be converted further on into a twelve by twelve $R(123,455)$ matrix: the three inactive isomers are excluded owing to the presence of the $\overline{55}$ chelating group, and the topological representation is that illustrated by Fig. 1 if one ignores the three central points.

$R(123,4\overline{55}) =$

	a	$\bar{b}$	c	$\bar{d}$	e	f	$\bar{a}$	b	$\bar{c}$	$\bar{d}$	$\bar{e}$	$\bar{f}$
a	0	0	1	0	1	2	0	1	0	1	0	0
$\bar{b}$	0	0	0	0	0	1	1	0	1	2	1	0
c	1	0	0	0	0	0	0	1	0	1	2	1
$\bar{d}$	0	0	0	0	0	1	1	2	1	0	1	0
e	1	0	0	0	0	0	0	1	2	1	0	1
f	2	1	0	1	0	0	0	0	1	0	1	0
$\bar{a}$	0	1	0	1	0	0	0	0	1	0	1	2
b	1	0	1	2	1	0	0	0	0	0	0	1
$\bar{c}$	0	1	0	1	2	1	1	0	0	0	0	0
d	1	2	1	0	1	0	0	1	0	0	0	1
$\bar{e}$	0	1	2	1	0	1	1	0	0	0	0	0
$\bar{f}$	0	0	1	0	1	0	1	1	0	0	1	0

The introduction of a $\overline{12}$ chelating group instead of a $\overline{55}$ one suppresses other isomers (f, $\bar{f}$, k). Fig. 2 shows how the hexagonal prism is then transformed into a pentagonal antiprism which can also be seen on matrix $R(\overline{123},455)$

$$R(\overline{123},455) = \begin{array}{c} \\ a \\ \bar{b} \\ c \\ \bar{d} \\ e \\ g \\ h \\ \bar{a} \\ b \\ \bar{c} \\ d \\ \bar{e} \end{array} \begin{array}{c} \begin{array}{cccccccccccc} a & \bar{b} & c & \bar{d} & e & g & h & \bar{a} & b & \bar{c} & d & \bar{e} \end{array} \\ \left[\begin{array}{cccccccccccc} 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 2 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 2 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}$$

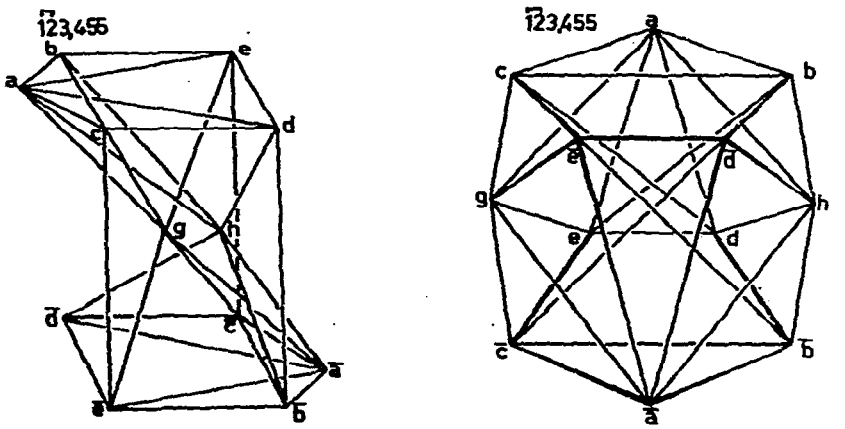

Fig. 2. Topological representations of the intramolecular isomerization reactions of $\overline{123},455$.

The introduction of two chelating groups gives a modified system with ten isomers.

$R(\overline{123},\overline{455})$ may easily be deduced from the constraint conditions[1] ($a=\bar{a}=f=\bar{f}=k=0$) and Fig. 3 describes this system topologically.

$$R(\overline{123},\overline{456}) = \begin{array}{c} \\ \bar{b} \\ c \\ \bar{d} \\ e \\ g \\ h \\ b \\ \bar{c} \\ d \\ \bar{e} \end{array} \begin{array}{c} \begin{array}{ccccccccccc} \bar{b} & c & \bar{d} & e & g & h & b & \bar{c} & d & \bar{e} \end{array} \\ \left[\begin{array}{cccccccccc} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 & \bar{1} \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}$$

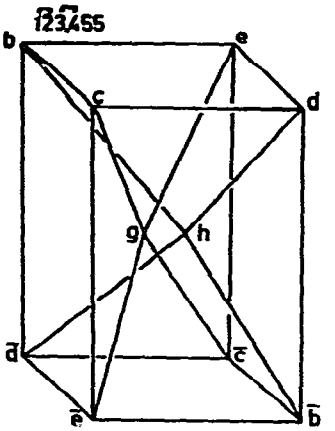

Fig. 3. Topological representation of the isomerization reactions of $\overline{123},455$.

The same may be done for $\overline{123},4\overline{55}$ [see matrix $R(\overline{123},4\overline{55})$ and Fig. 4]

$$R(\overline{123},4\overline{55}) = \begin{array}{c} \\ a \\ \bar{b} \\ c \\ \bar{d} \\ e \\ \bar{a} \\ b \\ \bar{c} \\ d \\ \bar{e} \end{array} \begin{array}{c} \begin{array}{ccccccccccc} a & \bar{b} & c & \bar{d} & e & \bar{a} & b & \bar{c} & d & \bar{e} \end{array} \\ \left[\begin{array}{cccccccccc} 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}$$

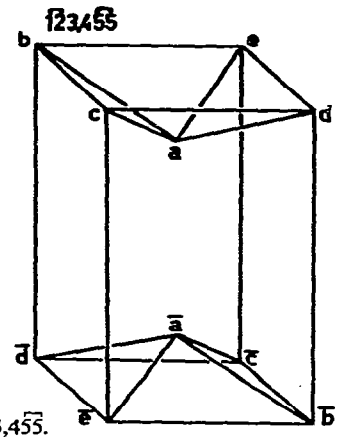

Fig. 4. Topological representation of the isomerization reactions of $\overline{123},4\overline{55}$.

The tris-chelate case $\overline{123},\overline{456}$, which has already been described[2], may be deduced from matrix $R(\overline{123},\overline{456})$ or from Fig. 3, by setting $g=h=0$, or from matrix $R(\overline{123},4\overline{55})$ or from Fig. 4 by setting $a=\bar{a}=0$.

$$R(\overline{123},\overline{455}) = \begin{array}{c} \\ \bar{b} \\ c \\ \bar{d} \\ e \\ b \\ \bar{c} \\ d \\ \bar{e} \end{array} \begin{array}{c} \begin{array}{ccccccccc} \bar{b} & c & \bar{d} & e & b & \bar{c} & d & \bar{e} \end{array} \\ \left[\begin{array}{cccccccc} 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 \\ 0 & 0 & 0 & 0 & 2 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 2 & 0 & 0 & 0 & 0 \\ 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}$$

123,456 systems

The representation of the general case (123,456), with 30 isomers and 120 isomerization paths, seems to require higher dimensionality and cannot be properly reduced for illustration. It should be a four-dimensional hypercube with 14 extra points.

The introduction of one chelating group suppresses six isomers and the reaction matrix for this case may be deduced from $R(123,456)$ by a suitable matrix transformation ($g=\bar{g}=k=\bar{k}=h=\bar{h}=0$ for $123,4\bar{5}\bar{6}$)

$R(123,4\bar{5}\bar{6}) =$

	a	b	c	d	e	f	i	j	l	m	n	q	$\bar{a}$	$\bar{b}$	$\bar{c}$	$\bar{d}$	$\bar{e}$	$\bar{f}$	$\bar{i}$	$\bar{j}$	$\bar{l}$	$\bar{m}$	$\bar{n}$	$\bar{q}$
a	0	0	1	0	1	1	1	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0
$\bar{b}$	0	0	0	0	0	1	0	0	0	0	0	0	1	0	1	1	0	0	0	1	1	0	0	0
c	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0	1	0	1	0	1	1	1	0	0
$\bar{d}$	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	1	0	0	0	0	1	1	0
e	1	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1	0	0	1	1	0	0
f	1	1	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	1	0	1	0
i	1	0	0	0	0	0	1	0	1	0	1	0	0	1	0	1	0	0	0	0	0	0	0	0
j	0	0	0	0	0	1	0	0	0	0	0	0	1	1	0	0	0	0	0	0	1	1	0	1
l	0	0	0	0	0	0	0	0	0	0	0	0	1	0	1	1	0	0	1	0	1	0	0	1
m	0	0	0	0	0	1	0	0	0	0	0	0	0	1	1	0	0	1	0	0	1	0	0	1
n	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	1	1	0	0	1	1	0
q	0	0	0	0	0	1	1	0	1	0	1	0	0	0	0	0	0	0	1	0	1	0	0	1
$\bar{a}$	0	1	0	1	0	0	0	0	0	0	0	0	0	0	1	0	1	1	1	0	0	0	0	0
b	1	0	1	1	0	0	0	1	1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
$\bar{c}$	0	1	0	0	1	0	1	1	1	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
d	1	1	0	0	1	0	0	0	0	1	1	0	0	0	0	0	0	0	1	0	0	0	0	0
$\bar{e}$	0	0	1	1	0	0	1	0	0	1	1	0	1	0	0	0	0	0	0	0	0	0	0	0
$\bar{f}$	0	0	0	0	0	0	0	0	1	0	1	0	1	1	0	1	0	0	0	0	0	0	0	1
$\bar{i}$	0	0	1	0	1	0	0	0	0	0	0	1	0	0	0	0	0	1	0	1	0	1	0	1
$\bar{j}$	0	1	1	0	0	0	0	1	1	0	1	0	0	0	0	0	0	0	1	0	0	0	0	0
$\bar{l}$	0	1	1	0	0	1	0	1	0	0	1	0	0	0	0	0	0	0	0	1	0	0	0	0
$\bar{m}$	0	0	0	1	1	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	1	0	0	0
$\bar{n}$	0	0	0	1	1	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0	1	0	0
$\bar{q}$	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	0	1	0	1	0	1	0

$R(12\bar{3},4\bar{5}\bar{6})$ may similarly be constructed from $R(123,4\bar{5}\bar{6})$ ($q=q=a=\bar{a}=0$).

$\hat{C}(f=\bar{f}=i=\bar{i}=0) \times R(12\bar{3},4\bar{5}\bar{6}) \times C(f=\bar{f}=i=\bar{i}=0)$ gives $R(\bar{1}2\bar{3},4\bar{5}\bar{6})^t$, which is the topological matrix of a four-dimensional hypercube. This corresponds to the topological[3] and matrix[4] descriptions given by Muetterties for this particular case.

$R(12\overline{3},\overline{456}) =$

	$\bar{b}$	c	$\bar{d}$	e	f	i	j	l	m	n	$b\bar{c}$	$d\bar{e}$	$\bar{f}\bar{i}$	$\bar{j}\bar{l}$	$\bar{m}\bar{n}$
$\bar{b}$	0	0	0	0	1	0	0	0	0	0	1	1	0	0	0
c	0	0	0	0	0	0	0	0	0	0	1	0	0	1	1
$\bar{d}$	0	0	0	0	1	0	0	0	0	0	1	0	0	1	0
e	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0
f	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0
i	0	0	0	0	0	1	0	1	0	0	1	0	1	0	0
j	0	0	0	0	1	0	0	0	0	1	1	0	0	0	0
l	0	0	0	0	0	0	0	0	0	0	1	1	0	0	1
m	0	0	0	0	1	0	0	0	0	0	1	1	0	0	1
n	0	0	0	0	0	0	0	0	0	0	0	1	1	1	0
b	0	1	1	0	0	0	1	1	0	0	0	0	0	1	0
$\bar{c}$	1	0	0	1	0	1	1	1	0	0	0	0	0	0	0
d	1	0	0	1	0	0	0	0	1	1	0	0	0	1	0
$\bar{e}$	0	1	1	0	0	1	0	0	1	1	0	0	0	0	0
$\bar{f}$	0	0	0	0	0	0	1	0	1	1	0	1	0	0	0
$\bar{i}$	0	1	0	1	0	0	0	0	0	0	0	0	0	1	0
$\bar{j}$	1	1	0	0	0	0	1	1	0	0	0	0	0	1	0
$\bar{l}$	1	1	0	0	1	0	1	0	0	1	0	0	0	0	0
$\bar{m}$	0	0	1	1	0	0	1	0	0	1	0	0	0	1	0
$\bar{n}$	0	0	1	1	1	0	0	1	1	0	0	0	0	0	0

$R(12\overline{3},\overline{434}) =$

	$\bar{b}$	c	e	l	$b\bar{c}$	$\bar{e}\bar{l}$	f	i	$\bar{f}$
$\bar{b}$	0	0	0	0	1	1	1	1	0
c	0	0	0	0	1	0	2	1	0
e	0	0	0	0	1	2	0	1	0
l	0	0	0	0	1	1	1	0	0
b	1	1	1	1	0	0	0	0	1
$\bar{c}$	1	0	2	1	0	0	0	0	1
$\bar{e}$	1	2	0	1	0	0	0	0	1
$\bar{l}$	1	1	1	0	0	0	0	1	0
f	1	0	0	0	0	0	0	0	1
i	0	1	1	0	0	1	0	0	0
$\bar{f}$	0	0	0	1	1	0	0	0	0

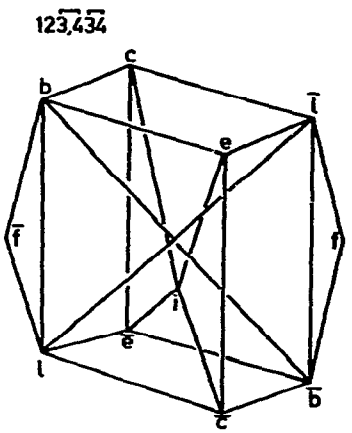

Fig. 5. Topological representation of the isomerization reactions of $12\overline{3},\overline{434}$.

123,344 and 113,344 systems

The only 123,344 system which has not yet been described[1,2] is that with unsymmetrical ligands: $12\overline{3},4\overline{3}4$. This case can be deduced[1] from $R(12\overline{3},4\overline{5}6)$ by setting $3=5$ and $4=6$. One gets[1] $b=d$, $c=m$, $e=j$, $l=n$, $\bar{b}=\bar{d}$, $\bar{c}=\bar{m}$, $\bar{e}=\bar{j}$, $\bar{l}=\bar{n}$, $i=\bar{i}$ (*i.e.* eleven isomers, f and $\bar{f}$ are unaffected by these constraints).

The topological description of this system is given in Fig. 5. It consists of a cube with two extra connections ($r_{b\bar{b}}=r_{l\bar{l}}=1$ instead of 0), with two twofold degenerate paths ($r_{c\bar{e}}=r_{\bar{c}e}=2$ instead of 1) and with three extra points (f, $\bar{f}$ and i).

The introduction of a third chelating group suppresses isomers i, f and $\bar{f}$, which gives

$$R(\overline{12\overline{3}},\overline{4\overline{3}4}) = \begin{array}{c} \\ \bar{b} \\ c \\ e \\ l \\ b \\ \bar{c} \\ \bar{e} \\ \bar{l} \end{array} \begin{array}{c} \begin{array}{cccccccc} \bar{b} & c & e & l & b & \bar{c} & \bar{e} & \bar{l} \end{array} \\ \left[\begin{array}{cccccccc} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 2 & 1 \\ 0 & 0 & 0 & 0 & 1 & 2 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}$$

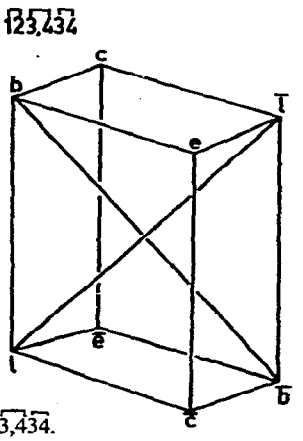

Fig. 6. Topological representation of the isomerization reactions of $\overline{12\overline{3}},\overline{4\overline{3}4}$.

If one sets $1=2$, one may reduce the former systems into $R(11\overline{3},4\overline{3}4)$ ($f=\bar{f}$, $b=\bar{l}$, $\bar{b}=l$) and $R(\overline{11}\overline{3},4\overline{3}4)$ ($b=\bar{l}$, $\bar{b}=1$) which leads to the following topoiogical representations (see Fig. 7):

$$R(11\overline{3},4\overline{3}4) = \begin{array}{c} \\ \bar{b} \\ c \\ e \\ f \\ i \\ b \\ \bar{c} \\ \bar{e} \end{array} \begin{array}{c} \begin{array}{ccccccc} \bar{b} & c & e & f & i & b & \bar{c} & \bar{e} \end{array} \\ \left[\begin{array}{ccccccc} 0 & 0 & 0 & 2 & 0 & 4 & 2 & 2 \\ 0 & 0 & 0 & 0 & 1 & 2 & 0 & 2 \\ 0 & 0 & 0 & 0 & 1 & 2 & 2 & 0 \\ 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 1 \\ 4 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 1 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 1 & 0 & 0 & 0 \end{array}\right] \end{array}$$

$$R(\overline{11}\overline{3},4\overline{3}4) = \begin{array}{c} \\ \bar{b} \\ c \\ e \\ b \\ \bar{c} \\ \bar{e} \end{array} \begin{array}{c} \begin{array}{cccccc} \bar{b} & c & e & b & \bar{c} & \bar{e} \end{array} \\ \left[\begin{array}{cccccc} 0 & 0 & 0 & 4 & 2 & 2 \\ 0 & 0 & 0 & 2 & 0 & 2 \\ 0 & 0 & 0 & 2 & 2 & 0 \\ 4 & 2 & 2 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 & 0 & 0 \end{array}\right] \end{array}$$

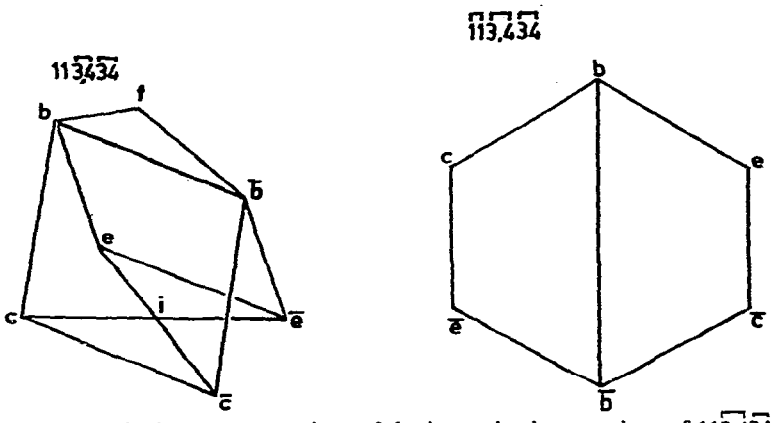

Fig. 7. Topological representations of the isomerization reactions of $11\overline{3},\overline{43}\overline{4}$ and $\overline{11}\overline{3},\overline{43}\overline{4}$.

ACKNOWLEDGEMENTS

The authors are indebted to Prof. J. Nasielski for helpfull discussions and valuable suggestions. They wish to thank Prof. R. Peretz and Ir. J. Giroul for appreciated help during the elaboration of the programms on a Bull General Electric computer. They express also their gratitude to the Institut pour l'encouragement de la Recherche Scientifique dans l'Industrie et l'Agriculture for the award of a fellowship (J.T.).

REFERENCES

1 M. GIELEN, G. MAYENCE AND J. TOPART, *J. Organometal. Chem.*, 18 (1969) 1.
2 M. GIELEN AND C. DEPASSE-DELIT, *Theor. Chim. Acta*, in press.
3 E. L. MUETTERTIES, *J. Amer. Chem. Soc.*, 90 (1968) 5097.
4 E. L. MUETTERTIES, *J. Amer. Chem. Soc.*, 91 (1969) in press.