the proof of theorem I in EPIR-I, eq A3 can be derived from eq A6.

As in EPIR-I, eq A7 is of interest.

$$F(W; 1, 1, ..., 1; 1, 1, ..., 1) = |W|^{-1} \sum_{w_i \in W} \left(\prod_{l=1}^{n_1} d_l ! l^{d_l}\right) \left(\prod_{u=1}^{n_2} e_u ! u^{e_u}\right)$$
(A7)

**C.** Theorem II. Theorem.— $B_1$ ,  $B_2$ , H, B, and W are defined as in theorem I. If  $D_W$  is the number of equivalency classes (double cosets  $Wh_iW$ ) generated in H when  $h_i$ ,  $h_j\epsilon$ H are considered equivalent if  $h_i = w_k \cdot h_j \cdot w_h$  for some  $w_k$ ,  $w_h\epsilon W$ , then

$$D_{\overline{W}} = |W|^{-2} \sum_{W}' (h_{d_1 d_2} \dots d_{n_1}, e_1 e_2 \dots e_{n_2})^2 \times \left( \prod_{l=1}^{n_1} d_l ! l^{d_l} \right) \left( \prod_{u=1}^{n_2} e_u ! u^{e_u} \right) \quad (A8)$$

where  $\Sigma'_W$  sums over the generalized cyclic types  $(d_1, d_2, \ldots, d_{n_1}; e_1, e_2, \ldots, e_{n_2})$  of operations in W and

 $h_{d_1d_2...d_{n_1},e_1e_2...e_{n_2}}$  is the number of operations in W of generalized cyclic type  $(d_1, d_2, ..., d_{n_1}; e_1, e_2, ..., e_{n_2})$ .

**Proof.**—This proof is not presented in detail since its course parallels the proof of theorem II in EPIR-I.

The group  $W^w$  acting on elements in H is defined as in EPIR-I. Then Burnside's Lemma implies

$$D_{\boldsymbol{W}} = |\boldsymbol{W}|^{-2} \sum_{(w_i, w_k) \in \boldsymbol{W}^{\boldsymbol{W}}} \boldsymbol{\chi}(w_i, w_k)$$
(A9)

where  $\chi(w_i, w_k)$  is the number of  $h_i$  in H which satisfy eq A10

$$h_i(w_k) = w_i \tag{A10}$$

Arguments used in EPIR-I show that eq A11 will hold if  $w_i$  and  $w_k$  are of the same cyclic type  $(d_1, d_2, \ldots, d_{n_1}; e_1, e_2, \ldots, e_{n_2})$ . If  $w_i$  and  $w_k$  are not of the

$$\chi(w_i, w_k) = \left(\prod_{l=1}^{n_1} d_l | l^{d_l}\right) \left(\prod_{u=1}^{n_2} e_u | u^{e_u}\right)$$
(A11)

same cyclic type,  $\chi(w_i, w_k) = 0$ . Equations A9 and A11 are combined as in EPIR-I to yield eq A8.

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## A Restatement of Polya's Theorem

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Polya's theorem is restated in a manner which may lead to greater ease of isomer enumeration and aid in the formulation of individual isomers. Several examples are treated.

A restatement of Polya's theorem in terms of invariance to covering operations may lead to a greater ease of isomer enumeration and aid in the formulation of the structure of individual isomers. The restatement<sup>1</sup> is as follows: the total number of (theoretically possible) stereoisomers of a molecule will be the number of distinguishable configurations of the molecule in a fixed coordinate system which are invariant under each operation of the rotational group (including the identity operation) divided by the total number of operations of the rotational group of the parent geometry. If the full covering group is used (*i.e.*, improper rotations are included) the result is the number of geometric isomers.

The distinguishable configurations invariant under the identity operation are simply the set of all distinguishable configurations, *i.e.*, the number of permutations of the ligands taken one at a time. The number of these depends only on the number of ligands of each type to be added and may be calculated from

$$P_1^n = \frac{n!}{n_{\rm e}! n_{\rm b}! n_{\rm e}! \dots}$$

(1) Although this restatement is essentially contained in one of Polya's original papers {Acta Mat. (Uppsala), **68**, 145 (1937)} the implications and simplifications have been overlooked in the recent literature concerned with isomers. A partial summary in English of this paper of Polya appears in a chapter by Uhlenbeck and Ford in "Studies in Statistical Mechanics," Vol. I, J. DeBoer and G. E. Uhlenbeck, Ed., Interscience, New York, N. Y. (North-Holland Publishing Co., Amsterdam), 1962.

where *n* is the total number of ligands,  $n_a$  is the number of A groups,  $n_b$  the number of B groups, etc. If only one ligand of each type is present ( $n_a = n_b = n_c = \ldots =$ 1) then  $P_1^n = n!$  and the total isomers possible will be n!/h where *h* is the order of the rotational group. This leads to the well-known (at least for the first few members) results shown in Table I.

MA	Table I ximum Number of Ste Given Parent G	REOISOMERS FOR A EOMETRY <sup>a</sup>
Coordin no.	Geometry and rotational group	No. of isomers
4	Tetrahedron $T$	4!/12 = 2
	Sq plane $D_4$	4!/8 = 3
	Sq pyr $C_4$	4!/4 = 6
	Boat $D_2$	4!/4 = 6
5	Trigonal bipyr $D_3$	5!/6 = 20
	Sq pyr $C_4$	5!/4 = 30
	Pentagon $C_5$	5!/10 = 12
6	Octahedron Q	6!/24 = 30
19	Icosahedron I	121/60 = 7.983.360

<sup>*a*</sup> Maximum achieved only when all ligands are different; planar geometries yield optically inactive isomers, and others give n/2 enantiomorphic pairs.

In order for a configuration to be invariant under a  $C_n$  operation, any ligands which do not fall on the  $C_n$  axis must be in sets of *n* similar ligands. Groups falling on the  $C_n$  axis belong to "sets of one." Each  $C_n$  opera-

TABLE II

TRANSFORMATIONS OF THE CONFIGURATIONS OF MenA<sub>2</sub>BC under the  $C_{2v}$  Operations

							1					1	$\leftrightarrow 2$				1 -	→ 1	
		Е	set		C2		3	$\leftrightarrow 4$		. 034		4			<b>T</b> 12		3 4	$\rightarrow 4$	
Configura-										Position of ligar	1d			-,					
tion no.	1	2	3	4		1	- 2	3	4		1	2	3	4		1	2	3	4
1	в	¢	$\mathbf{A}$	Α	4	С	в	Α	Á	4	C	в	Ą	Α	. 1	в	С	Á	Α
2	в	Α	С	À	6	Α	È	Α	C	5	A	в	С	Α	3	в	Α	Α	C
3	в	A	Α	С	5	Α	в	C.	Α	6	Ά	в	Α	С	2	в	Α	С	A
4	С	в	Α	Α	1 ,	в	С	Α	Α	1	в	C	Α	A	4	С	в	Α	Α
5	Α	В	С	Α	3	в	Α	Α	С	<b>2</b>	в	Α	C	Α	6	Α	в	Â	С
6	Α	в	Α	С	<b>2</b>	в	Α	C	Α	3	B	Α	Α	С	5	A	в	С	A
7	С	Α	в	А	11	Α	С	Α	в	8	Ά	С	в	Á	10	С	Α	Α	в
8	Α	С	в	Α	10	С	Α	Α	в	7	С	Α	в	Á	11	Α	С	A	в
9	Α	Α	В	С	12	Α	A	С	в	9	Α	Α	В	C	12	A	Α	С	в
10	С	Α	А	в	8	A	С	в	Α	11	Ä	C	Α	в	. 7	С	Α	в	Α
11	Α	Ċ	Α	в	7	С	Α	в	Α	10	С	Α	Α	B	8	Α	С	в	Α
12	Α	Α	С	в	9	Á	Α	·B	С	12	A	Α	С	в	9	Á	Α	в	С

tion will thus have associated with it a permutation function of the form  $P_n^m$  or  $P_1^k P_n^m$  where nm + k =total number of ligands. Here  $P_n^m$  is the number of permutations of ligands distributed into *m* sets of *n* similar ligands and may be calculated from

$$P_n^m = \frac{m!}{n_{\mathbf{a}_n}!n_{\mathbf{b}_n}!n_{\mathbf{c}_n}!\dots}$$

where  $n_{a_n}$  is the number of sets of  $A_n$ ,  $n_{b_n}$  is the number of sets of  $B_n$ , and  $n_{a_n} + n_{b_n} + \ldots = m$ . The  $P_1^k$  may be evaluated in a fashion identical with that for  $P_1^n$ , *i.e.* 

$$P_1^k = \frac{k!}{n_{\rm s}! n_{\rm b}! n_{\rm c}! \dots}$$

where  $n_{\rm a} + n_{\rm b} + \ldots = k$ .

In evaluating  $P_1^k P_n^m$  in cases where  $P_1^k$  and  $P_n^m$  are not independent (as with  $P_1^2 P_2^2$  for A<sub>4</sub>B<sub>2</sub>), all possibilities must be evaluated and summed (1 + 2 in the case cited).

The permutation functions  $P_n^m$  are identical in form with the  $f_n^m$  functions which appear in Polya's cycle index.<sup>2</sup> The  $f_n^m$  functions were to be evaluated by the expansion of  $(A^n + B^n + C^n + \ldots)^m$ . Product functions  $f_1^k f_n^m$  were to be evaluated by the expansion of  $(A + B + C + \ldots)^k (A^n + B^n + C^n + \ldots)^m$ . The value of a particular value of  $P_1^k P_n^m$  is the coefficient of the appropriate  $A^x B^y C^z$ ... term in the expansion where x, y, and z are the stoichiometric subscripts of  $MA_x B_y C_z$ ... of the compound of interest. It is obvious that particular  $P_n^m$  permutation functions are identical with the corresponding coefficients of the polynomial expansion and that inspection of the  $f_1^k f_n^m$ expansion allows rapid identification of "all possibilities" of  $P_1^k P_n^m$  to be evaluated.

**Some Examples.**—Some simple examples will be considered first to illustrate the method with verifiable solutions.

Consider the problem: How many isomers are possible for  $MenA_2BC$  where en is a bidentate chelate group, M is the central metal, and the geometry is taken as octahedral?

Chelates are not yet well handled by Polya's method so the Men unit is considered as the "parent" and the point group is thus  $C_{2v}$ .



CHART I

No. of stereoisomers = 
$$\frac{1}{2}[12 + 0] = 6$$
  
No. of geometric isomers =  $\frac{1}{4}[12 + 0 + 2 + 2] = 4$   
No. of  $dl$  pairs =  $6 - 4 = 2$ 

To formulate these isomers we return to Polya's expansion of the  $f_1^n$  term, but in order not to lose information we multiply step by step, *i.e.* 

$$f_1^4 = (A_1 + B_1 + C_1)(A_2 + B_2 + C_2) \times (A_3 + B_3 + C_3)(A_4 + B_4 + C_4)$$

and collect the  $A^{2}BC$  terms as shown in Table II under the E set. The  $C_2$  operation causes the subscript changes  $1 \rightarrow 2, 2 \rightarrow 1, 3 \rightarrow 4, 4 \rightarrow 3$ . The  $C_2$  operation on the E set produces a rearranged E set since no configurations are invariant under  $C_2$ . Since configuration  $1 \rightarrow 4$  under rotation, these two configurations arise from the same isomer and either may be used to represent it. In this fashion the six stereoisomers may be readily identified as 1, 2, 3, 7, 8, and 9. The  $\sigma_{12}$ operation leaves subscripts 1 and 2 unchanged but interchanges 3 and 4;  $\sigma_{34}$  gives  $3 \rightarrow 3, 4 \rightarrow 4, 1 \rightarrow 2$ ,  $2 \rightarrow 1$ . Optically inactive isomers are invariant under  $\sigma$  (or in general under  $S_n$  operations); the  $\sigma$  operation on an optically active isomer will produce its enantiomer. Thus we identify configurations 1 and 9 as inactive and 2 and 3 and 7 and 8 as dl pairs.

The application of Polya's method to isomer formulation may be seen to be essentially the process which chemists have been using intuitively all along, *i.e.*, all possible configurations are considered and duplicates are eliminated by seeing which configurations may be

<sup>(2)</sup> These have been tabulated for a variety of geometries for both the rotational group and the full covering group by B. A. Kennedy, D. A. McQuarrie, and C. H. Brubaker, Jr., *Inorg. Chem.*, **3**, 265 (1964).

brought into coincidence through rotation.<sup>3</sup> Polya's method ensures that no possible configurations are overlooked and that all rotational operations of the parent group are considered. It is obvious that in formulating isomers one need not carry out the rotational transformations for all rotations if the number of unique formulations of isomers is found earlier. It is also obvious that only one transformation needs to be carried out to determine dl pairs and optically inactive isomers.

Restriction of Coordination Sites.—A problem posed, and solved, by Kennedy, McQuarrie, and Brubaker will be used to illustrate the treatment of restricted coordination sites, *i.e.*, how many isomers are possible for Nb<sub>2</sub>Cl<sub>2</sub>(OC<sub>2</sub>H<sub>5</sub>)<sub>6</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>2</sub> if the basic geometry consists of two octahedrally coordinated Nb atoms bridged by Cl and/or OC<sub>2</sub>H<sub>5</sub> at two sites and with one C<sub>5</sub>H<sub>5</sub>N attached to each Nb atom?



The restrictions are readily incorporated in Polya's method by the manner of expansion of the cyclic index (or by the way the cyclic indices are formulated).



No. of stereoisomers =  $\frac{1}{4}[448 + 16 + 16] = 120$ <sup>a</sup> A = Cl, B = OC<sub>2</sub>H<sub>5</sub>, and C = C<sub>5</sub>H<sub>5</sub>N.

Note that for one pyridine molecule on each Nb atom an invariant configuration under a  $C_2^{\nu}$  operation cannot be written so the  $f_1^2 f_2^4$  term is zero for this operation. More appropriately, the  $C_2^{\nu}$  operation yields an  $f_1^2 f_2^2 f_2^2$  term, the  $f_2^{2^*}$ s to be evaluated for each Nb. The  $f_1^2$  terms are to be interpreted as arising from the bridge positions, and in expansions of the polynomials, only A and B go into this term; or, alternatively, for the  $C_2^x$  and  $C_2^z$  operations if A is on the bridge there are 4!/3! ways to attach the two C's to achieve invariance under the  $C_2$ ; if B is on the bridge then the two A's and two C's may be attached in 4!/2! ways to achieve invariance under the  $C_2$  operations.

(3) See W. E. Bennett, Inorg. Chem., 8, 1325 (1969), for a Fortran program for the octahedral case and a general discussion.

TABLE III ISOMERS OF B<sub>12</sub>F<sub>6</sub>H<sub>6</sub><sup>2-</sup>

Highest proper

The number of geometric isomers is obtained from the full symmetry group and Polya's method. Three additional terms (Chart III) appear due to the three reflection planes present, and the inversion center yields the last term. The  $f_1^2$  or  $f_2^1$  terms arise from the bridging position and hence are restricted to A and/or B. The  $(f_1^2f_1^2)$  term represents the ligands in the mirror plane—to be invariant under  $\sigma xy$  or  $\sigma yz$  the C's must be in the mirror plane.



Figure 1.—(a) View down 1–12  $C_5$  axis. (b) View down 1, 2, 3  $C_3$  axis. (c) View down  $C_2$  through 1, 2 and 9, 12 edges.

or

01

 $\begin{array}{ccc} (A+B)^2(A+B+C)^2(A+B+C)^2(A^2+B^2)^2 = \dots 32A^2B^6C^2\\ \sigma yz \longrightarrow f_2^{-1}(f_1^2f_1^2)f_2^2 \longrightarrow 16 \text{ (evaluated as with the first three terms above)} \end{array}$ 

$$(A^{2} + B^{2})(A + B + C)^{2}(A + B + C)^{2}(A^{2} + B^{2})^{2} \longrightarrow$$

 $...16A^{2}B^{6}C^{2}$ 

$$\begin{array}{c} \sigma xz \longrightarrow J_1 t_2 z^* \\ (A_2)(B_6C_2) \longrightarrow 4!/3! \longrightarrow 4 \\ (B_2)(A_2B_4C_2) \longrightarrow 4!/2! \longrightarrow 12 \\ (AB)(AB_5C_2) \longrightarrow 0 \end{array}$$

. . . .

or

 $(A + B)^{2}(A^{2} + B^{2} + C^{2})^{4} \longrightarrow \dots 16A^{2}B^{4}C^{2}$   $i \longrightarrow f_{2}!f_{2}^{4}$   $(A_{2})(B_{6}C_{2}) \longrightarrow 4!/3! \longrightarrow 4$   $(B_{2})(A_{2}B_{4}C_{2}) \longrightarrow 4!/2! \longrightarrow 12$ 



No. of geometrical isomers = 2160/120 = 18No. of stereoisomers = 1440/60 = 24No. of dl pairs = 6

From the above the number of geometric isomers = 1/8[480 + 32 + 16 + 16] = 70. Number of *dl* pairs = 120 - 70 = 50.

These results are, of course, in agreement with those of Kennedy, *et al.*, as well as those of Block and Maguire<sup>4</sup> who have used a different approach.

(4) B. P. Block and K. D. Maguire, Inorg. Chem., 6, 2107 (1967).

Isomers of the Icosahedral Borate Anion.—The application of Polya's theorem to the determination of the number of isomers of  $B_{12}F_6H_6^{2-}$  is straightforward but the formulation of these isomers by the examination of the *E* set of configurations for duplicates under a rotation from each class of the covering group would require a computer or a saint! Nevertheless, Polya's theorem provides sufficient aid that, with a little organization, these isomers may readily be deduced.

 $B_{12}F_6H_6^{2-}$  Isomers.—Haas<sup>5</sup> has enumerated the isomers of all  $B_{10}H_{10-n}X_n^{2-}$  and  $B_{12}H_{12-n}X_n^{2-}$  anions by Polya's method and formulated them by an undisclosed procedure. We examine here the  $B_{12}H_6F_6^{2-}$ isomers and several more complex cases to illustrate the use of Polya's method in isomer formulation. These isomers have not been renumbered to produce the lowest sum (as is correctly done in the work of Haas) since the symmetry is less readily visualized on renumbering.

The covering operations of the iocosahedron (the parent geometry of  $B_{12}F_6H_6{}^{2-}$ ), the related permutation functions, and the numerical evaluation of the configurations invariant under these operations, along with the number of isomers for  $B_{12}F_6H_6{}^{2-}$ , are given in Chart IV.

The permutation functions under the rotational operations tell us (note this information was initially used to construct the permutation functions) that under a

20.5

20P.2

 $15\sigma$ 

 $15P_1^4P_2^4$ 

15(8 + 36)

 $12S_{10}$   $12S_{10}^{3}$ 

 $24P_2 P_{10}$ 

0

61

3131

 $C_5$  operation two unique positions fall on the  $C_5$  axis (points 1 and 12 Figure 1) and two unique sets of five exist (2-6 and 7-11). There are four ways of filling these positions with six ligands for a given  $C_5$  axis to produce configurations which are invariant under the  $C_5$  operation (Chart V).

(5) T. E. Haas, *ibid.*, **3**, 1053 (1964) [the use of a computer was not mentioned].

					Сн	ART	v					
	1	2	3	4	5	6	7	8	9	10	11	12
(a)	F	F	F	F	F	F						
(b)		$\mathbf{F}$					$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	F	F	
(c)		$\mathbf{F}$	F	$\mathbf{F}$	$\mathbf{F}$	F						$\mathbf{F}$
(d)							F	F	F	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$

Configurations (c) and (d) arise from the same isomers as (a) and (b) as a  $C_2$  operation about any  $C_2$  axis  $\perp$  to the chosen  $C_5$  axis carries (c) into (a) and (d) into (b). These isomers and a graphical representation are shown in Table III.

In similar fashion the  $P_3^4$  function arising from the  $C_3$  operation indicates that under a  $C_3$  operation four unique sets of three exist (see Figure 1), and there are six configurations achieving invariance under a  $C_3$  operation with six positions filled (Chart VI).

## CHART VI

	1	2	3	4	6	7	5	8	11	9	10	12
(e)	F	F	F	F	F	F						
(f)	$\mathbf{F}$	$\mathbf{F}$	F				$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$			
(g)	F	$\mathbf{F}$	F							$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$
(h)				$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$			
(i)				$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$				$\mathbf{F}$	F	$\mathbf{F}$
(j)							F	$\mathbf{F}$	F	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$

Since a  $C_2$  operation about a  $C_2$  axis perpendicular to the  $C_3$  axis carries 1 2 3 into 9 10 12 and 4 6 7 into 5 8 11 only (g) and (h) are invariant under this  $C_2$  operation, (j) going into (e) and (i) into (f). These four isomers arise from the set invariant under the  $C_3$  operation.

The  $P_2^6$  function arising from the  $C_2$  operation gives rise to 20 configurations invariant under this  $C_2$  (see Figure 1).

CHART VII

	• = =												
	1	2	3	6	4	11	5	7	8	10	9	12	
( <b>k</b> )	F	$\mathbf{F}$	F	F	F	F							
(1)	F	$\mathbf{F}$	F	$\mathbf{F}$			$\mathbf{F}$	F					
(m)	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$					$\mathbf{F}$	$\mathbf{F}$			
(n)	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$							F	F	
(o)	F	$\mathbf{F}$			$\mathbf{F}$	$\mathbf{F}$	F	$\mathbf{F}$					
(p)	F	F			$\mathbf{F}$	$\mathbf{F}$			$\mathbf{F}$	$\mathbf{F}$			
(q)	F	F			$\mathbf{F}$	F					F	F	
( <b>r</b> )	F	$\mathbf{F}$					$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$			
(s)	F	F					$\mathbf{F}$	$\mathbf{F}$			F	$\mathbf{F}$	
(t)	$\mathbf{F}$	$\mathbf{F}$							F	F	F	F	
(u)			$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	F	$\mathbf{F}$					
$(\mathbf{v})$			F	F	$\mathbf{F}$	$\mathbf{F}$			$\mathbf{F}$	$\mathbf{F}$			
(w)			$\mathbf{F}$	$\mathbf{F}$	F	F					F	$\mathbf{F}$	
(x)			$\mathbf{F}$	$\mathbf{F}$			F	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$			
(y)			F	F			F	$\mathbf{F}$			F	$\mathbf{F}$	
(z)			$\mathbf{F}$	$\mathbf{F}$					$\mathbf{F}$	$\mathbf{F}$	F	$\mathbf{F}$	
(aa)					$\mathbf{F}$	$\mathbf{F}$	F	F	$\mathbf{F}$	$\mathbf{F}$			
(bb)					$\mathbf{F}$	F	F	$\mathbf{F}$			F	$\mathbf{F}$	
(cc)					F	$\mathbf{F}$			F	$\mathbf{F}$	$\mathbf{F}$	$\mathbf{F}$	
(dd)							F	F	$\mathbf{F}$	F	F	F	

A  $C_2$  operation about the  $C_2$  axis through the 4, 5 and 7, 11 edges brings about the transformations

$$1, 2 \leftrightarrow 9, 12$$
$$3, 6 \leftrightarrow 8, 10$$
$$4, 11 \leftarrow 5, 7$$

Hence, configurations (k) and (dd) arise from the same isomer as do (l) and (cc), (m) and (z), (n) and (t), etc. Removal of the isomers already counted as invariant under  $C_3$  reduces the number of new isomers found here to eight of which four may readily be seen to be optically inactive and the remainder to consist of 2 *dl* pairs. These are listed along with their maps in Table III.

There remain six geometric isomers to be found which have no rotational axis beyond the  $C_1$  axis. These may be found by moving one F position from among the isomers already found in such a fashion as to remove all rotational symmetry or simply to produce a new mapping. The 1 2 3 4 5 6 isomer is thus the parent of the first four geometric isomers listed under  $C_1$  while the 1 2 3 5 8 11 isomer is respectively parent and grandparent of the remaining two.

**Isomers of B**<sub>12</sub>**H**<sub>6</sub>**F**<sub>5</sub>**X**<sup>2-</sup>.—To find the isomers of B<sub>12</sub>**H**<sub>6</sub>**F**<sub>5</sub>**X**<sup>2-</sup>, we replace one F with X in each unique manner. The F<sub>6</sub> set invariant under  $C_5$  yields two F<sub>5</sub>X isomers for each F<sub>6</sub> isomer; those invariant under  $C_3$  alone also yield two F<sub>5</sub>X isomers for each F<sub>6</sub> isomer, while those invariant under both a  $C_3$  and a  $C_2$  operation yield a single F<sub>5</sub>X isomer for each F<sub>6</sub> isomer; those invariant under  $C_1$  alone yield three F<sub>5</sub>X isomers for each F<sub>6</sub> isomer; those invariant under  $C_2$  alone yield three F<sub>5</sub>X isomers for each F<sub>6</sub> isomer; those invariant under  $C_2$  alone yield three F<sub>5</sub>X isomers for each F<sub>6</sub> isomer; those invariant under  $C_1$  only yield six F<sub>5</sub>X isomers for each F<sub>6</sub> isomer. These isomers total 94 for B<sub>12</sub>H<sub>6</sub>F<sub>5</sub>X<sup>2-</sup> in agreement with the number calculated by Polya's theorem for an icosahedral B<sub>12</sub> framework. These may be written by inspection with the aid of maps such as in Table III.

**Isomers of B**<sub>12</sub>H<sub>5</sub>F<sub>5</sub>X<sub>2</sub><sup>2-</sup>.—Polya's theorem leads to the possibility of 12 geometrical and 14 stereoisomers for B<sub>12</sub>H<sub>7</sub>F<sub>5</sub><sup>2-</sup> and these have been formulated by Haas. To find the 278 isomers possible for B<sub>12</sub>H<sub>5</sub>F<sub>5</sub>X<sub>2</sub><sup>2-</sup> we note that the only parent F<sub>5</sub> grouping invariant under the  $C_5$  operation has a mapping of  $\bigcirc$  leaving a mapping of  $\bigotimes$  for the H<sub>7</sub> grouping. Substitution of two X groups in this  $C_{5v}$  parent map leads to five isomers which may be written by inspection. The remaining 13 stereoisomers belong only to the  $C_1$  set and hence the two X groups may be distributed among the parent H<sub>7</sub> positions in 7!/5!2!, or 21, ways. These may be written without difficulty, *i.e.*, for the 1, 2, 3, 4, 5 B<sub>12</sub>H<sub>7</sub>F<sub>5</sub><sup>2-</sup> parent



For  $B_{12}H_6F_4X_2^{2-}$  we expect 246 isomers. Using the  $F_6$  mapping of Table III we find three under each parent  $C_5$  set, five under each  $C_3$  set, three under each  $D_3$  set (*i.e.*,  $C_8$  set with  $\perp C_2$ ), nine under each  $C_2$  set, and 15 under each  $C_1$  set.