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Group Theoretical Classification of Solutions of the Unrestricted Hartree-Fock Equation in Molecular Systems with a Spatial Point Symmetry

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A group theoretical classification of solutions of the UHF equation is developed for molecular systems with a spatial point symmetry. All possible types of UHF solutions with distinct broken symmetries are listed up for each spatial point symmetry group P. It is shown that a UHF solution of torsional spin wave (TSW) type is characterized by a subgroup P' of P, its normal subgroup N, its factor group $F=P'/N$ and an automorphism of F. The condition is given for a UHF solution of TSW type to be admissible with each of the other seven classes in spin and time reversal symmetry. An algorism is given to obtain the spin structure which is realizable in a UHF solution.

§ 1. Introduction

In a previous paper[1] (hereafter referred to as II), one of the authors developed a theory for classification and characterization of solutions of the UHF (unrestricted Hartree-Fock) equation. The theory is based on the fact that the symmetry operations to leave a UHF solution invariant form a subgroup of the symmetry group G_0 of the system, and all possible types of UHF solutions with distinct broken symmetries can be exhausted by listing up all inequivalent subgroups of G_0.

It was shown in II that UHF solutions in any electron system with the symmetry for the group S of spin rotations and the group T of the time reversal are classified into the eight distinct classes corresponding to the eight inequivalent subgroups of the group $G_0=S\times T$. The classification given in II is applicable to any non-relativistic electron system with a spin independent Hamiltonian.

However, many molecular systems have a group $\boldsymbol{P}$ of a spatial point symmetry and then it is possible to extend the classification of UHF solutions further. It has been shown that the HF ground state of chemically reacting molecules may undergoes "phase" transitions between UHF solutions with different spin structures and the spin structures of the HF "phases" may be of plentiful varieties but are closely correlated with the spatial symmetry of the system.[2] Therefore, it is of chemical interest, not mathematical, to study what kinds of UHF solutions are possible in a system with a spatial point symmetry.

In the present paper, we develop a group theoretical classification of UHF solutions in a system with the symmetry group $G_0=\boldsymbol{P}\times S\times T$ by applying the above-mentioned principle. We shall show that all subgroups of G_0 can be constructed from the subgroups of TSW (torsional spin wave) type which have no element belonging to $S\times T$ and are 'generalized magnetic double groups' which may be a magnetic group or a double group[3] in some special cases. We shall list up all the subgroups of TSW type for each point symmetry group. The condition is obtained for such a subgroup to be admissible with the other seven classes in spin and time reversal symmetry. We use the same notations as those in the previous papers.[1),4)]

§ 2. Preliminaries

In the following, we consider a system with the symmetry group $G_0=\boldsymbol{P}\times S\times T$, where $\boldsymbol{P}$ is a spatial point symmetry group, S is the group of spin rotations and T is the group of order two consisting of the time reversal t and the unit element E. We denote the elements of $\boldsymbol{P}$ by p. The elements u of S are 2×2 unitary unimodular matrices. We denote the element of S corresponding to the rotation around an axis $\boldsymbol{e}$ by θ radian as $u(\boldsymbol{e},\theta)$. The element $u(\boldsymbol{e},2\pi)=-\mathbf{1}$ is independent of $\boldsymbol{e}$ and denoted by $\bar{E}$.

The symmetry operations to leave the Slater determinant $\Psi=\|\phi_\alpha\|$ of a UHF solution invariant (except for the phase) form a subgroup G of G_0 which we call the invariance group of Ψ. Then the conjugate subgroup $G^{(g)}=gGg^{-1}$ by any $g\in G_0$ is the invariance group of the UHF solution $g\Psi=\|g\phi_\alpha\|$, and $g\Psi$ has the same Hartree-Fock energy as Ψ. Hence, the members of the set of the UHF solutions $\{g\Psi|g\in G_0\}$ are physically equivalent and the subgroups conjugate to G correspond to the same physical state as G. As the relation of the conjugation of subgroups is an equivalence relation (we denote it by $\sim$) , we can decompose the set $\boldsymbol{S}(G_0)$ of all the subgroups of G_0 into equivalence classes according to this equivalence relation, and we obtain a quotient set $\boldsymbol{Q}(G_0)=\boldsymbol{S}(G_0)/\sim$. The quotient set $\boldsymbol{Q}(G_0)$ represents physically distinct types of UHF solutions. Our aim is to list up all representative subgroups of the equivalence classes in $\boldsymbol{Q}(G_0)$.

We consider all point groups as $\boldsymbol{P}$. However, as there are some isomorphisms among point groups, it is sufficient to consider only the groups which are not mutually isomorphic. Hereafter we use the Schönflies notation[3] for point groups and their elements. There are the following isomorphisms between point groups,[5] $\boldsymbol{C}_{2m}\simeq\boldsymbol{S}_{2m}\simeq\boldsymbol{C}_{mh}$ for odd m, except that $\boldsymbol{S}_2$ usually replaced by the symbol $\boldsymbol{C}_I$, $\boldsymbol{C}_{2m}\simeq\boldsymbol{S}_{2m}$ for even m, $\boldsymbol{D}_n\simeq\boldsymbol{C}_{nv}$ for odd n, $\boldsymbol{D}_{2m}\simeq\boldsymbol{C}_{2mv}\simeq\boldsymbol{D}_{mh}\simeq\boldsymbol{D}_{md}$ for odd m, $\boldsymbol{D}_{2m}\simeq\boldsymbol{C}_{2mv}\simeq\boldsymbol{D}_{md}$ for even m, $\boldsymbol{O}\simeq\boldsymbol{T}_d$, $\boldsymbol{D}_2\simeq\boldsymbol{C}_{2h}\simeq\boldsymbol{C}_{2v}$ and $\boldsymbol{D}_\infty\simeq\boldsymbol{C}_{\infty v}$. Hence, we consider only the following point groups, $\boldsymbol{C}_n$, $\boldsymbol{D}_n$, $\boldsymbol{T}$, $\boldsymbol{O}$, $\boldsymbol{C}_{nh}$ (even n), $\boldsymbol{D}_{nh}$ (even n), $\boldsymbol{C}_\infty$, $\boldsymbol{C}_{\infty h}$, $\boldsymbol{D}_\infty$ and $\boldsymbol{D}_{\infty h}$.

§ 3. Subgroups of TSW type

A subgroup of G_0 is called TSW type and denoted as $G_{\rm TSW}$ if it does not contain any pure spin rotation or spin rotation combined with the time reversal. That is, any element ($\neq E$) of $S\times T$ is contained in $G_{\rm TSW}$ only in a form coupled with an element $p(\neq E)\in\boldsymbol{P}$, or equivalently, $G_{\rm TSW}$ consists of the spatial symmetry operations $p\in\boldsymbol{P}$ coupled with some elements of $S\times T$. The set of $p\in\boldsymbol{P}$ contained in $G_{\rm TSW}$ forms a subgroup $\boldsymbol{P}'$ of $\boldsymbol{P}$. For the time being, we consider only such $G_{\rm TSW}$'s that contain all the elements of $\boldsymbol{P}$. In the case of $G_{\rm TSW}$ involving only the elements of a subgroup $\boldsymbol{P}'$ of $\boldsymbol{P}$, we can start from $\boldsymbol{P}'$ instead of $\boldsymbol{P}$ without changing the following arguments. As $G_{\rm TSW}$ is a group consisting of the spatial symmetry operations $p\in\boldsymbol{P}$ coupled with some elements of $S\times T$, it is written as

$$G_{\rm TSW}=\{pr(p)\,|p\in\boldsymbol{P},r(p)\in S\times T\}. \tag{3·1}$$

The necessary and sufficient condition for (3·1) to be a group is that for any $p_1,p_2\in\boldsymbol{P}$, if $p_1p_2=p_3$, then $r(p_1)r(p_2)=r(p_3)$ or $r(p_3)\bar{E}$. This implies that r must be a homomorphism of $\boldsymbol{P}$ into $S\times T/{}_{II}\boldsymbol{C}_1$, where ${}_{II}\boldsymbol{C}_1=\{E,\bar{E}\}$.

A homomorphism of $\boldsymbol{P}$ into $S\times T/{}_{II}\boldsymbol{C}_1$ is constructed as follows. Let h be a group homomorphism of $\boldsymbol{P}$ into $\boldsymbol{O}(3)$. The image $h(\boldsymbol{P})$ is a subgroup of $\boldsymbol{O}(3)$. We next make a one to two mapping of $h(\boldsymbol{P})$ into $S\times T$. A proper rotation $q=h(p)$ in $h(\boldsymbol{P})$ is mapped to the spin rotation $u(q)$ with the axis and angle of rotation the same as q. An improper rotation $q'=h(p')$ in $h(\boldsymbol{P})$ which is a product $q'=Iq$ of the inversion I and a proper rotation q is mapped to the product $tu(q)$ of the time reversal t and the spin rotation $u(q)$. We denote the obtained image of $p\in\boldsymbol{P}$ in $S\times T$ as $\bar{h}(p)$. The set $\{h(p)\,|p\in\boldsymbol{P}\}$, however, is not a subgroup of $S\times T$ but the set ${}_{II}h(\boldsymbol{P})=\{\bar{h}(p),\bar{h}(p)\bar{E}|p\in\boldsymbol{P}\}$ doubled with $\bar{E}$ is a subgroup because of the one to two correspondence of $\boldsymbol{SO}(3)$ and $S=\boldsymbol{SU}(2)$ groups. A subgroup of TSW type is obtained by the coupling of $p\in\boldsymbol{P}$ with the elements $\bar{h}(p)$ and $\bar{h}(p)\bar{E}$ in $S\times T$:

$${}_{II}\boldsymbol{P}_h=\{p\bar{h}(p),p\bar{h}(p)\bar{E}|p\in\boldsymbol{P}\}. \tag{3·2}$$

We note that the groups with the structure (3·2) include as the special cases the double groups and the magnetic groups constructed from $\boldsymbol{P}$ and may be called 'generalized magnetic double groups'. We use the Roman left suffix II to indicate that the group is a kind of magnetic double group. The group ${}_{II}\boldsymbol{P}_h$ is specified by a homomorphism h of $\boldsymbol{P}$ into $\boldsymbol{O}(3)$.

By isomorphism theorem, the homomorphic image $h(\boldsymbol{P})$ is isomorphic to the factor group $\boldsymbol{F}=\boldsymbol{P}/\boldsymbol{N}\subset\boldsymbol{O}(3)$ where $\boldsymbol{N}$ is the kernel of h and a normal subgroup of $\boldsymbol{P}$. As a consequence of this theorem all types of homomorphic mappings of $\boldsymbol{P}$ are obtained by considering all normal subgroups $\boldsymbol{N}$ of $\boldsymbol{P}$ and their factor groups $\boldsymbol{F}=\boldsymbol{P}/\boldsymbol{N}$. Therefore, by listing up all normal subgroups $\boldsymbol{N}$ and its factor groups $\boldsymbol{F}$, we can list up all subgroups of TSW type constructed from $\boldsymbol{P}$. In the same manner as the mapping of $h(p)$ to $\bar{h}(p)$, we can map elements f of $\boldsymbol{F}$ to the elements $\bar{f}$ in $S\times T$. Let us factorize $\boldsymbol{P}$ into the left cosets with respect to $\boldsymbol{N}$; $\boldsymbol{P}=\sum_f p_f \boldsymbol{N}$, where p_f are the representatives of the left cosets with a one to one correspondence to the elements f of $\boldsymbol{F}$. Then, the group (3·2) can be specified by $\boldsymbol{N}$ and $\boldsymbol{F}$ instead of h and represented as

$$_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F}) = \{p_f\boldsymbol{N}\bar{f},\, p_f\boldsymbol{N}\bar{f}\bar{E}\,|\,f\in\boldsymbol{F}\}. \qquad (3\cdot 3)$$

We list up in Tables I and II all proper normal subgroups of all the point groups under consideration and their factor groups $\boldsymbol{F}$. $\boldsymbol{P}$ and $\boldsymbol{E}$ are always normal subgroups of P, and not listed in these tables. We note that as a result of the presence of some isomorphisms among point groups, we can take as a factor group

Table I. Proper normal subgroups and factor groups of finite point groups.

$\boldsymbol{P}$	$\boldsymbol{N}$	$\boldsymbol{F}$	comment
$\boldsymbol{C}_n$	$\boldsymbol{C}_p$	$\boldsymbol{C}_{n/p}$	p: divisor of n
$\boldsymbol{D}_n(n:\text{odd})$	$\boldsymbol{C}_p$	$\boldsymbol{D}_{n/p}$	p: divisor of n
$\boldsymbol{D}_{2m}(m\neq 1)$	$\boldsymbol{D}_m$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_p$	$\boldsymbol{D}_{2m/p}$	p: divisor of $2m$
$\boldsymbol{D}_2$	$\boldsymbol{C}_{2x}$	$\boldsymbol{C}_2$	$\boldsymbol{C}_{2x}=(E, C_{2x})$
	$\boldsymbol{C}_{2y}$	$\boldsymbol{C}_2$	$\boldsymbol{C}_{2y}=(E, C_{2y})$
	$\boldsymbol{C}_{2z}$	$\boldsymbol{C}_2$	$\boldsymbol{C}_{2z}=(E, C_{2z})$
$\boldsymbol{T}$	$\boldsymbol{D}_2$	$\boldsymbol{C}_3$	
$\boldsymbol{O}$	$\boldsymbol{D}_2$	$\boldsymbol{D}_3$	
	$\boldsymbol{T}$	$\boldsymbol{C}_2$	
$\boldsymbol{C}_{2mh}$	$\boldsymbol{C}_p\times\boldsymbol{C}_I$	$\boldsymbol{C}_{2m/p}$	p: divisor of $2m$
	$\boldsymbol{C}_p$	$\boldsymbol{C}_{2m/p}\times\boldsymbol{C}_I$	p: divisor of $2m$
	$\boldsymbol{C}_{p/2}+I\boldsymbol{C}_p^{1}\boldsymbol{C}_{p/2}$	$\boldsymbol{C}_{4m/p}$	p: divisor of $2m$
$\boldsymbol{D}_{2mh}$	$\boldsymbol{D}_{2m}$	$\boldsymbol{C}_2$	
	$\boldsymbol{D}_m\times\boldsymbol{C}_I$	$\boldsymbol{C}_2$	
	$\boldsymbol{D}_m+IC^1_{2m}\boldsymbol{D}_m$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_{2m}\times\boldsymbol{C}_I$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_{2m}+IC_{2x}\boldsymbol{C}_{2m}$	$\boldsymbol{C}_2$	
	$\boldsymbol{D}_m$	$\boldsymbol{C}_2\times\boldsymbol{C}_I$	
	$\boldsymbol{C}_{2m}$	$\boldsymbol{C}_2\times\boldsymbol{C}_I$	
	$\boldsymbol{C}_m\times\boldsymbol{C}_I$	$\boldsymbol{D}_2$	
	$\boldsymbol{C}_m+IC_{2x}\boldsymbol{C}_m$	$\boldsymbol{D}_2$	
	$\boldsymbol{C}_m+IC^1_{2m}\boldsymbol{C}_m$	$\boldsymbol{D}_2$	
	$\boldsymbol{C}_m$	$\boldsymbol{D}_2\times\boldsymbol{C}_I$	
	$\boldsymbol{C}_p\times\boldsymbol{C}_I$	$\boldsymbol{D}_{2m/p}$	p: divisor of $2m$
	$\boldsymbol{C}_p$	$\boldsymbol{D}_{2m/p}\times\boldsymbol{C}_I$	p: divisor of $2m$
	$\boldsymbol{C}_{p/2}+IC_p^{1}\boldsymbol{C}_{p/2}$	$\boldsymbol{D}_{2m/p}\times\boldsymbol{C}_I$	p: even, divisor of $2m$

Table II. Proper normal subgroups and factor groups of compact point groups.

$\boldsymbol{P}$	$\boldsymbol{N}$	$\boldsymbol{F}$	comment
$\boldsymbol{C}_\infty$	$\boldsymbol{C}_p$	$\boldsymbol{C}_\infty$	$p=2,3,\cdots$
$\boldsymbol{C}_{\infty h}$	$\boldsymbol{C}_\infty$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_p\times\boldsymbol{C}_I$	$\boldsymbol{C}_\infty$	$p=1,2,\cdots$
	$\boldsymbol{C}_p$	$\boldsymbol{C}_{\infty h}$	$p=2,3,\cdots$
	$\boldsymbol{C}_p+IC_{2p}^1\boldsymbol{C}_p$	$\boldsymbol{C}_{\infty h}$	$p=1,2,\cdots$
$\boldsymbol{D}_\infty$	$\boldsymbol{C}_\infty$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_p$	$\boldsymbol{D}_\infty$	$p=2,3,\cdots$
$\boldsymbol{D}_{\infty h}$	$\boldsymbol{D}_\infty$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_{\infty v}$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_{\infty h}$	$\boldsymbol{C}_2$	
	$\boldsymbol{C}_\infty$	$\boldsymbol{C}_2\times\boldsymbol{C}_I$	
	$\boldsymbol{C}_p+IC_{2x}\boldsymbol{C}_p$	$\boldsymbol{C}_{\infty h}$	$p=1,2,\cdots$
	$\boldsymbol{C}_p\times\boldsymbol{C}_I$	$\boldsymbol{D}_\infty$	$p=1,2,\cdots$
	$\boldsymbol{C}_p$	$\boldsymbol{D}_{\infty h}$	$p=2,3,\cdots$

$\boldsymbol{F}$ any one of groups isomorphic to $\boldsymbol{F}$. Hence there are different ways of the coupling of a point symmetry with an element of $S\times T$ with the same number as that of the point groups isomorphic to $\boldsymbol{F}$.

Furthermore, there may be the other type of the coupling, because there are automorphisms in a factor group $\boldsymbol{F}$. By an automorphism $\boldsymbol{A}: f\in\boldsymbol{F}\rightarrow\boldsymbol{A}(f)\in\boldsymbol{F}$, we can construct from ${}_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F})$ of (3·3) another subgroup as follows;

$${}_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F},\boldsymbol{A}) = \{p_f\boldsymbol{N}\bar{\boldsymbol{A}}(f),\, p_f\boldsymbol{N}\bar{\boldsymbol{A}}(f)E \mid f\in\boldsymbol{F}\}, \tag{3·4}$$

where $\bar{\boldsymbol{A}}(f)$ is the element of $S\times T$ corresponding to $\boldsymbol{A}(f)$. However, the subgroups obtained by inner automorphisms $\boldsymbol{g}^\#$ (that is, the automorphisms defined by $\boldsymbol{g}^\#(f)=g^{-1}fg, g\in\boldsymbol{O}(3)$) are mutually conjugate and represent the same physical state as $\boldsymbol{F}$. We derive here a prescription to get the outer automorphisms leading to distinct physical states. For the time being, we regard $\boldsymbol{F}$ as a subgroup of $\boldsymbol{O}(3)$. We denote the group of all automorphisms of $\boldsymbol{F}$ by $\boldsymbol{A}(F)$ and the normalizer and centralizer groups of $\boldsymbol{F}$ in $\boldsymbol{O}(3)$ by $\boldsymbol{H}(\boldsymbol{F})$ and $\boldsymbol{Z}(\boldsymbol{F})$, respectively. Then, we have the following theorems.

Theorem 1. $\boldsymbol{Z}(\boldsymbol{F})$ is a normal subgroup of $\boldsymbol{H}(\boldsymbol{F})$ and the group $\boldsymbol{I}(\boldsymbol{F})$ of all inner automorphisms of $\boldsymbol{F}$ is represented as

$$\boldsymbol{I}(\boldsymbol{F}) = \boldsymbol{H}(\boldsymbol{F})/\boldsymbol{Z}(\boldsymbol{F}). \tag{3·5}$$

Theorem 2. In the decomposition of the group of automorphisms $\boldsymbol{A}(\boldsymbol{F})$ into right cosets with respect to $\boldsymbol{I}(\boldsymbol{F})$;

$$\boldsymbol{A}(\boldsymbol{F}) = \sum_\alpha \boldsymbol{I}(\boldsymbol{F})\boldsymbol{t}_\alpha, \tag{3·6}$$

Table III. Centralizer groups $\boldsymbol{Z}(\boldsymbol{F})$, normalizer groups $\boldsymbol{H}(\boldsymbol{F})$ and $\boldsymbol{I}(\boldsymbol{F})=\boldsymbol{H}(\boldsymbol{F})/\boldsymbol{Z}(\boldsymbol{F})$ of factor groups $\boldsymbol{F}$.

$\boldsymbol{F}$	$\boldsymbol{Z}(\boldsymbol{F})$	$\boldsymbol{H}(\boldsymbol{F})$	$\boldsymbol{I}(\boldsymbol{F})$
$\boldsymbol{C}_n$ and $\boldsymbol{C}_n\times\boldsymbol{C}_I$ $(n\neq1,2)$	$\boldsymbol{C}_{\infty h}$	$\boldsymbol{D}_{\infty h}$	$\boldsymbol{C}_2\cong(\boldsymbol{E},\boldsymbol{C}_{2x}^{\#})$
$\boldsymbol{D}_n$ and $\boldsymbol{D}_n\times\boldsymbol{C}_I$ $(n\neq1,2)$	$\boldsymbol{C}_{2h}$	$\boldsymbol{D}_{2nh}$	$\boldsymbol{D}_n\cong\{(\boldsymbol{C}_{2n}^{+i})^{\#},(\boldsymbol{C}_{2x}\boldsymbol{C}_{2n}^{+i})^{\#}\}$ $i=0,1,2,\cdots,n-1$
$\boldsymbol{C}_2$ and $\boldsymbol{C}_{2h}$	$\boldsymbol{D}_{\infty h}$	$\boldsymbol{D}_{\infty h}$	$\boldsymbol{C}_1$
$\boldsymbol{D}_2$ and $\boldsymbol{D}_{2h}$	$\boldsymbol{D}_{2h}$	$\boldsymbol{O}_h$	$\boldsymbol{D}_3\cong\{\boldsymbol{E},\boldsymbol{C}_{31}^{+\#},\boldsymbol{C}_{31}^{-\#},\boldsymbol{C}_{2d}^{\#},(\boldsymbol{C}_{31}^{+}\boldsymbol{C}_{2d})^{\#},(\boldsymbol{C}_{31}^{-}\boldsymbol{C}_{2d})^{\#}\}$
$\boldsymbol{T}$ and $\boldsymbol{T}_h$	$\boldsymbol{C}_I$	$\boldsymbol{O}_h$	$\boldsymbol{O}\cong\{\boldsymbol{g}^{\#}\mid g\in\boldsymbol{O}\}$
$\boldsymbol{O}$ and $\boldsymbol{O}_h$	$\boldsymbol{C}_I$	$\boldsymbol{O}_h$	$\boldsymbol{O}\cong\{\boldsymbol{g}^{\#}\mid g\in\boldsymbol{O}\}$
$\boldsymbol{C}_\infty$ and $\boldsymbol{C}_{\infty h}$	$\boldsymbol{C}_{\infty h}$	$\boldsymbol{D}_{\infty h}$	$\boldsymbol{C}_2\cong(\boldsymbol{E},\boldsymbol{C}_{2x}^{\#})$
$\boldsymbol{D}_\infty$ and $\boldsymbol{D}_{\infty h}$	$\boldsymbol{C}_{2h}$	$\boldsymbol{D}_{\infty h}$	$\boldsymbol{D}_\infty\cong\{\boldsymbol{C}(\theta)^{\#},(\boldsymbol{C}_{2x}\boldsymbol{C}(\theta))^{\#}\}$ $0\leqq\theta\leqq\pi$

Table IV. Generators and their defining relations of finite point groups.

$\boldsymbol{P}$	generators	defining relations
$\boldsymbol{C}_n$	$a=C_n^{+}$	$a^n=E$
$\boldsymbol{D}_n$	$a=C_n^{+},b=C_{2x}$	$a^n=E,b^2=E$ and $bab=a^{-1}$
$\boldsymbol{T}$	$a=C_{31}^{+}$, $b=C_{2x}$, $c=C_{2z}$	$a^3=E$, $b^2=E$, $c^2=E$, $ba=ac$, $cb=bc$ and $ca=abc$
$\boldsymbol{O}$	$a=C_{31}^{+}$, $b=C_{2x}$, $c=C_{2z}$ and $d=\sigma_{dd}$	$a^3=E$, $b^2=E$, $c^2=E$, $d^2=E$, $ba=ac$, $cb=bc$, $ca=abc$, $da=a^2cd$, $db=bd$ and $dc=bcd$
$\boldsymbol{S}_{2m}$ $(m:\text{odd})$	$a=C_m^{+}$ and $b=I$	$a^m=E$, $b^2=E$ and $ab=ba$
$\boldsymbol{C}_{2mh}$	$a=C_{2m}^{+}$ and $b=I$	$a^{2m}=E$, $b^2=E$ and $ab=ba$
$\boldsymbol{D}_{md}$ $(m:\text{odd})$	$a=C_m^{+}$, $b=C_{2x}$ and $c=I$	$a^m=E$, $b^2=E$, $c^2=E$, $bab=a^{-1}$, $ac=ca$ and $bc=cb$
$\boldsymbol{D}_{2mh}$	$a=C_{2m}^{+}$, $b=C_{2x}$ and $c=I$	$a^{2m}=E$, $b^2=E$, $c^2=E$, $bab=a^{-1}$, $ac=ca$ and $bc=cb$

there is a one to one correspondence between the right cosets and the physically distinct automorphisms.

We give proofs of Theorems 1 and 2 in Appendices 1 and 2. From these theorems, we can find the physically distinct automorphisms. We list up $\boldsymbol{Z}(\boldsymbol{F})$, $\boldsymbol{H}(\boldsymbol{F})$ and $\boldsymbol{I}(\boldsymbol{F})$ for each point group in Table III. We cannot present any general formula of $\boldsymbol{A}(\boldsymbol{F})$. Then $\boldsymbol{A}(\boldsymbol{F})$ must be obtained individually for each $\boldsymbol{F}$.

An automorphism of $\boldsymbol{F}$ is determined by a transformation of the generators to the other generators which satisfy the same defining relation as the original generators. We list up in Table IV the generators and their defining relations in each point symmetry group.

(1) $\boldsymbol{C}_n$ $(n>2)$

Let us denote the natural numbers which are smaller than n and relatively prime to n by $p_1(n)=1,p_2(n),\cdots p_{e(n)}(n)$, where $e(n)$ is the Euler function of n. Then there are the following automorphisms in $\boldsymbol{C}_n$,

$$\boldsymbol{A}_i(a)=a^{p_i(n)};\quad i=1,2,\cdots e(n). \tag{3·7}$$

Because $\boldsymbol{I}(\boldsymbol{C}_n)$ is $(\boldsymbol{E},\boldsymbol{C}_{2x}^{\#})$ and $\boldsymbol{C}_{2x}^{\#}(a)=C_{2x}^{-1}C_n^{+}C_{2x}=C_n^{-1}=a^{-1}=a^{n-1}$, $\boldsymbol{A}_i$ and $\boldsymbol{A}_{e(n)-i+1}$

with $i \leqq e(n)/2$ are mutually transferred by an inner automorphism. Hence

$$\boldsymbol{A}(\boldsymbol{C}_n)/\boldsymbol{I}(\boldsymbol{C}_n) = \{\boldsymbol{A}_i | i=1, 2, \cdots e(n)/2\}, \tag{3·8}$$

and the number of physically distinct automorphisms is $e(n)/2$.

(2) $\boldsymbol{D}_n$ $(n>2)$

$\boldsymbol{A}(\boldsymbol{D}_n)$ consists of the following $ne(n)$ transformations of the generators;

$$\boldsymbol{A}_{i,j}(a, b) = (a^{p_i(n)}, ba^j); j=0, 1, \cdots n-1, i=1, 2, \cdots e(n). \tag{3·9}$$

Hence

$$\boldsymbol{A}(\boldsymbol{D}_n)/\boldsymbol{I}(\boldsymbol{D}_n) = \{\boldsymbol{A}_{i,0} | i=1, \cdots e(n)/2\}. \tag{3·10}$$

(3) $\boldsymbol{T}$

$\boldsymbol{A}(\boldsymbol{T})$ consists of the following 24 transformations of the generators.

$$\boldsymbol{A}_{i,j} = \psi_j \phi_i, \quad \boldsymbol{A}'_{i,j} = \psi_j' \phi_i'; \quad i=1, 2, 3, 4, \ j=1, 2, 3, \tag{3·11}$$

where ϕ_i, ψ_j, ϕ_i' and ψ_j' are the following transformations of the generators;

$$\left.\begin{array}{l} \phi_1: a \to a, \ \phi_2: a \to ab, \ \phi_3: a \to ac, \ \phi_4: a \to abc, \\ \phi_1': a \to a^2, \ \phi_2': a \to a^2 b, \ \phi_3': a \to a^2 c, \ \phi_4': a \to a^2 bc, \\ \psi_1: b \to b, \ c \to c, \ \psi_2: b \to c, \ c \to bc, \ \psi_3: b \to bc, \ c \to b, \\ \psi_1': b \to b, \ c \to bc, \ \psi_2': b \to c, \ c \to b, \ \psi_3': b \to bc, \ c \to c. \end{array}\right\} \tag{3·12}$$

As the order of $\boldsymbol{I}(\boldsymbol{T})$ is 24, $\boldsymbol{A}(\boldsymbol{T})/\boldsymbol{I}(\boldsymbol{T})$ is $\boldsymbol{C}_1$.

(4) $\boldsymbol{O}$

In this case, though it is more troublesome to obtain $\boldsymbol{A}(\boldsymbol{O})$, we can see that $\boldsymbol{A}(\boldsymbol{O})/\boldsymbol{I}(\boldsymbol{O}) = \boldsymbol{C}_1$ by a manner similar to the case of $\boldsymbol{T}$.

(5) $\boldsymbol{S}_{2m} = \boldsymbol{C}_m \times \boldsymbol{C}_I$ $(m$: odd)

$\boldsymbol{A}(\boldsymbol{S}_{2m})$ consists of

$$\boldsymbol{A}_i(a, b) = (a^{p_i(n)}, b); i=, \cdots e(n). \tag{3·13}$$

As in the case (1), $\boldsymbol{A}_i$ and $\boldsymbol{A}_{e(n)-i+1}$ with $i \leqq e(n)/2$ are mutually transferred by an inner automorphism, and we obtain

$$\boldsymbol{A}(\boldsymbol{S}_{2m})/\boldsymbol{I}(\boldsymbol{S}_{2m}) = \{\boldsymbol{A}_i | i=1, \cdots e(n)/2\}. \tag{3·14}$$

(6) $\boldsymbol{C}_{2mh} = \boldsymbol{C}_{2m} \times \boldsymbol{C}_I$

$\boldsymbol{A}(\boldsymbol{C}_{2mh})$ consists of

$$\left.\begin{array}{ll} \boldsymbol{A}_i^{(1)}(a, b) = (a^{p_i(2m)}, b), & \boldsymbol{A}_i^{(2)}(a, b) = (a^{p_i(2m)}, a^m b), \\ \boldsymbol{A}_i^{(3)}(a, b) = (ba^{p_i(2m)}, b), & \boldsymbol{A}_i^{(4)}(a, b) = (ba^{p_i(2m)}, a^m b), \end{array}\right\} \tag{3·15}$$

where $i=1, \cdots e(2m)$. Hence, $\boldsymbol{A}(\boldsymbol{C}_{2mh})/\boldsymbol{I}(\boldsymbol{C}_{2mh})=\{\boldsymbol{A}_i^{(1)}, \boldsymbol{A}_i^{(2)}, \boldsymbol{A}_i^{(3)}, \boldsymbol{A}_i^{(4)} | i \leqq e(2m)/2\}$.

(7) $\boldsymbol{D}_{md}=\boldsymbol{D}_m \times \boldsymbol{C}_I$ (m: odd)

$\boldsymbol{A}(\boldsymbol{D}_{md})$ consists of

$$\left.\begin{aligned} \boldsymbol{A}_{i,k}^{(1)}(a, b, c) &= (a^{p_i(m)}, a^k b, c), \\ \boldsymbol{A}_{i,k}^{(2)}(a, b, c) &= (a^{p_i(m)}, a^k bc, c), \end{aligned}\right\} \tag{3·16}$$

where $i=1, \cdots e(m)$ and $k=0, \cdots, m-1$. Hence $\boldsymbol{A}(\boldsymbol{D}_{md})/\boldsymbol{I}(\boldsymbol{D}_{md})$ is $\{\boldsymbol{A}_{i,0}^{(1)}, \boldsymbol{A}_{i,0}^{(2)} | i \leqq e(m)/2\}$.

(8) $\boldsymbol{D}_{2mh}=\boldsymbol{D}_{2m} \times \boldsymbol{C}_I$

$\boldsymbol{A}(\boldsymbol{D}_{2mh})$ consists of

$$\left.\begin{aligned} \boldsymbol{A}_{i,k}^{(1)}(a, b, c) &= (a^{p_i(2m)}, a^k b, c), \\ \boldsymbol{A}_{i,k}^{(2)}(a, b, c) &= (a^{p_i(2m)}, a^k b, a^m c), \\ \boldsymbol{A}_{i,k}^{(3)}(a, b, c) &= (a^{p_i(2m)}, a^k bc, c), \\ \boldsymbol{A}_{i,k}^{(4)}(a, b, c) &= (a^{p_i(2m)}, a^k bc, a^m c), \\ \boldsymbol{A}_{i,k}^{(5)}(a, b, c) &= (ca^{p_i(2m)}, a^k b, c), \\ \boldsymbol{A}_{i,k}^{(6)}(a, b, c) &= (ca^{p_i(2m)}, a^k b, a^m c), \\ \boldsymbol{A}_{i,k}^{(7)}(a, b, c) &= (ca^{p_i(2m)}, ca^k b, c), \\ \boldsymbol{A}_{i,k}^{(8)}(a, b, c) &= (ca^{p_i(2m)}, ca^k b, a^m c), \end{aligned}\right\} \tag{3·17}$$

where $i=1, \cdots, e(m)$ and $k=0, \cdots, 2m-1$. Hence $\boldsymbol{A}(\boldsymbol{D}_{2mh})/\boldsymbol{I}(\boldsymbol{D}_{2mh}) = \{\boldsymbol{A}_{i,0}^{(t)} | t=1, \cdots, 8$ and $i \leqq e(2m)/2\}$.

(9) $\boldsymbol{C}_2$

It is obvious that $\boldsymbol{A}(\boldsymbol{C}_2)/\boldsymbol{I}(\boldsymbol{C}_2)=\boldsymbol{C}_1$.

(10) $\boldsymbol{D}_2$

$\boldsymbol{A}(\boldsymbol{D}_2)$ consists of the six permutations of a, b and ab. They are just the inner automorphisms by the elements of $\boldsymbol{I}(\boldsymbol{D}_2)$. Hence, $\boldsymbol{A}(\boldsymbol{D}_2)/\boldsymbol{I}(\boldsymbol{D}_2)=\boldsymbol{C}_1$.

(11) $\boldsymbol{C}_{2h}=\boldsymbol{C}_2 \times \boldsymbol{C}_I$

$\boldsymbol{A}(\boldsymbol{C}_{2h})$ consists of the six permutations of a, b and ab. Hence $\boldsymbol{A}(\boldsymbol{C}_{2h})/\boldsymbol{I}(\boldsymbol{C}_{2h}) = \boldsymbol{A}(\boldsymbol{C}_{2h})$.

(12) $\boldsymbol{D}_{2h}=\boldsymbol{D}_2 \times \boldsymbol{C}_I$

$\boldsymbol{A}(\boldsymbol{D}_{2h})$ is obtained as follows. We can choose as a any one from the seven elements of $\boldsymbol{D}_{2h}$ except for E and as b any one from the remaining six elements and as c any one from the four residual elements except for ab and E. Hence $\boldsymbol{A}(\boldsymbol{D}_{2h})$ consists of $7 \times 6 \times 4=168$ elements and $\boldsymbol{A}(\boldsymbol{D}_{2h})/\boldsymbol{I}(\boldsymbol{D}_{2h})$ of $168/6=28$ elements.

(13) $\boldsymbol{C}_\infty$

$\boldsymbol{A}(\boldsymbol{C}_\infty)$ consists of the following automorphisms;

$$A_1: C(\phi) \to C(\phi)\,,\ \ A_2: C(\phi) \to C(-\phi)\,. \tag{3·18}$$

Hence $\boldsymbol{A}(\boldsymbol{C}_\infty)/\boldsymbol{I}(\boldsymbol{C}_\infty) = \boldsymbol{C}_1$.

(14) $\boldsymbol{C}_{\infty h} = \boldsymbol{C}_\infty \times \boldsymbol{C}_I$

$\boldsymbol{A}(\boldsymbol{C}_{\infty h})/\boldsymbol{I}(\boldsymbol{C}_{\infty h})$ consists of the following two automorphisms:

$$A_1:\ (C(\phi)\,, I) \to (C(\phi)\,, I)\,, A_2:\ (C(\phi)\,, I) \to (C(\phi)\,, IC(\pi))\,. \tag{3·19}$$

(15) $\boldsymbol{D}_\infty$

$\boldsymbol{A}(\boldsymbol{D}_\infty)$ consists of the following mappings:

$$A_0(C(\phi)\,, C_{2x}) = (C(\phi)\,, C_{2x}C(\theta))\,,$$
$$A_0'(C(\phi)\,, C_{2x}) = (C(-\phi)\,, C_{2x}C(\theta))\,, \tag{3·20}$$

where $0 \leqq \theta \leqq \pi$. Hence, $\boldsymbol{A}(\boldsymbol{D}_\infty)/\boldsymbol{I}(\boldsymbol{D}_\infty) = \boldsymbol{C}_1$.

(16) $\boldsymbol{D}_{\infty h} = \boldsymbol{D}_\infty \times \boldsymbol{C}_I$

It is easy to see that $\boldsymbol{A}(\boldsymbol{D}_{\infty h})/\boldsymbol{I}(\boldsymbol{D}_{\infty h})$ consists of the following automorphisms:

$$A_1(C(\phi)\,, C_{2x}, I) = (C(\phi)\,, C_{2x}, I)\,,$$
$$A_2(C(\phi)\,, C_{2x}, I) = (C(\phi)\,, C_{2x}, C(\pi)\,I)\,,$$
$$A_3(C(\phi)\,, C_{2x}, I) = (C(\phi)\,, C_{2x}I, I)\,,$$
$$A_4(C(\phi)\,, C_{2x}, I) = (C(\phi)\,, C_{2x}I, C(\pi)\,I)\,. \tag{3·21}$$

Thus we have obtained all inequivalent automorphisms of $\boldsymbol{F}$.

We show here some examples of the subgroups of TSW type.

Example 1) $\boldsymbol{P} = \boldsymbol{C}_6$

In this case, there are the following normal subgroups, $\boldsymbol{N}_1 = \boldsymbol{C}_1$, $\boldsymbol{N}_2 = \boldsymbol{C}_2$, $\boldsymbol{N}_3 = \boldsymbol{C}_3$ and $\boldsymbol{N}_4 = \boldsymbol{C}_6$, and the corresponding factor groups are $\boldsymbol{F}_1 = \boldsymbol{C}_6/\boldsymbol{C}_1 = \boldsymbol{C}_6 \simeq \boldsymbol{S}_6 \simeq \boldsymbol{C}_{3h}$, $\boldsymbol{F}_2 = \boldsymbol{C}_2 \simeq \boldsymbol{C}_I \simeq \boldsymbol{C}_{1h}$ and $\boldsymbol{F}_4 = \boldsymbol{C}_1$. For these factor groups, all of $\boldsymbol{A}(\boldsymbol{F})/\boldsymbol{I}(\boldsymbol{F})$ are $\boldsymbol{C}_1$, then we have the subgroups of TSW type as follows:

$$G_{\mathrm{TSW}_1} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_1, \boldsymbol{C}_6, \boldsymbol{E}) = \{u(e_z, 2\pi i/6)\ (E, \overline{E})\, C_6^{\,i} \,|\, i = 0, \cdots, 5\}\,,$$

$$G_{\mathrm{TSW}_2} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_1, \boldsymbol{S}_6, \boldsymbol{E}) = {}_{II}\boldsymbol{C}_3(\boldsymbol{C}_1, \boldsymbol{C}_3, \boldsymbol{E}) + tC_2^{\,1}{}_{II}\boldsymbol{C}_3(\boldsymbol{C}_1, \boldsymbol{C}_3, \boldsymbol{E})\,,$$

$$G_{\mathrm{TSW}_3} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_1, \boldsymbol{C}_{3h}, \boldsymbol{E}) = {}_{II}\boldsymbol{C}_3(\boldsymbol{C}_1, \boldsymbol{C}_3, \boldsymbol{E}) + tu(e_z, \pi)\, C_2^{\,1}{}_{II}\boldsymbol{C}_3(\boldsymbol{C}_1, \boldsymbol{C}_3, \boldsymbol{E})\,,$$

$$G_{\mathrm{TSW}_4} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_2, \boldsymbol{C}_3, \boldsymbol{E}) = \boldsymbol{C}_2 \times {}_{II}\boldsymbol{C}_3(\boldsymbol{C}_1, \boldsymbol{C}_3, \boldsymbol{E})\,,$$

$$G_{\mathrm{TSW}_5} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_3, \boldsymbol{C}_2, \boldsymbol{E}) = \boldsymbol{C}_3(E, \bar{E}) + C_2^1 u(e_z, \pi)\, \boldsymbol{C}_3(E, \bar{E}),$$

$$G_{\mathrm{TSW}_{5'}} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_3, \boldsymbol{C}_2', \boldsymbol{E}) = \boldsymbol{C}_3(E, \bar{E}) + C_2^1 u(e_x, \pi)\, \boldsymbol{C}_3(E, \bar{E}),$$

$$G_{\mathrm{TSW}_6} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_3, \boldsymbol{C}_I, \boldsymbol{E}) = \boldsymbol{C}_3(E, \bar{E}) + tC_2^1 \boldsymbol{C}_3(E, \bar{E}),$$

$$G_{\mathrm{TSW}_7} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_3, \boldsymbol{C}_{1h}, \boldsymbol{E}) = \boldsymbol{C}_3(E, \bar{E}) + tu(e_z, \pi)\, C_2^1 \boldsymbol{C}_3(E, \bar{E}),$$

$$G_{\mathrm{TSW}_8} = {}_{II}\boldsymbol{C}_6(\boldsymbol{C}_6, \boldsymbol{C}_1, \boldsymbol{E}) = \boldsymbol{C}_6(E, \bar{E}),$$

where the $\boldsymbol{E}$ in ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{E})$ is the identity automorphism. It should be noted that G_{TSW_2}, G_{TSW_3}, G_{TSW_6} and G_{TSW_7} are the magnetic groups of the second kind. $G_{\mathrm{TSW}_{5'}}$ is conjugate to G_{TSW_5}.

Example 2) $\boldsymbol{P} = \boldsymbol{C}_5$

The normal subgroups in this case are $\boldsymbol{N}_1 = \boldsymbol{C}_1$ and $\boldsymbol{N}_2 = \boldsymbol{C}_5$, and the corresponding factor groups are $\boldsymbol{F}_1 = \boldsymbol{C}_5$ and $\boldsymbol{F}_2 = \boldsymbol{C}_1$. For $\boldsymbol{F}_1 = \boldsymbol{C}_5$, as there are two inequivalent outer automorphisms; $\boldsymbol{A}_1(a) = a$ and $\boldsymbol{A}_2(a) = a^2$, we have

$$G_{\mathrm{TSW}_1} = {}_{II}\boldsymbol{C}_5(\boldsymbol{C}_1, \boldsymbol{C}_5, \boldsymbol{A}_1) = \{C_5^i u(e_z, 2\pi i/5)\, (E, \bar{E})\,;\, i = 0, \cdots, 4\},$$

$$G_{\mathrm{TSW}_2} = {}_{II}\boldsymbol{C}_5(\boldsymbol{C}_1, \boldsymbol{C}_5, \boldsymbol{A}_2) = \{C_5^i u(e_z, 2\times 2\pi i/5)\, (E, \bar{E})\,;\, i = 0, \cdots, 4\}.$$

For $\boldsymbol{F}_2 = \boldsymbol{C}_1$, we have

$$G_{\mathrm{TSW}_3} = {}_{II}\boldsymbol{C}_5(\boldsymbol{C}_5, \boldsymbol{C}_1, \boldsymbol{E}) = \boldsymbol{C}_5(E, \bar{E}).$$

Here we describe a procedure for constructing the spin structure invariant to the group ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{A}) = \{p_f n \bar{\boldsymbol{A}}(f), p_f n \bar{\boldsymbol{A}}(f) \bar{E} \mid f \in \boldsymbol{F}, n \in \boldsymbol{N}\}$. We call a position vector $\boldsymbol{R}$ a general position vector[6] of a molecule if $p\boldsymbol{R} \neq p'\boldsymbol{R}$ for any $p \neq p' \in \boldsymbol{P}$. Let us call a spin vector $\boldsymbol{S}(\boldsymbol{R})$ at $\boldsymbol{R}$ a general spin vector for ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{E})$ if $\bar{f}\boldsymbol{S}(\boldsymbol{R}) \neq \bar{f}'\boldsymbol{S}(\boldsymbol{R})$ for any $f \neq f'$, where f and f' are elements of the union of $\boldsymbol{F}$ and all $\boldsymbol{F}'$s (if exist) isomorphic to $\boldsymbol{F}$. Then a spin structure invariant to ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{A})$ is obtained by applying all elements of ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{A})$ to a general spin vector $\boldsymbol{S}(\boldsymbol{R})$ at a general position vector $\boldsymbol{R}$. Then the spin structure is the set of the spin vectors $\{\bar{\boldsymbol{A}}(f)\, \boldsymbol{S}(p_f n \boldsymbol{R}) \mid f \in \boldsymbol{F}, n \in \boldsymbol{N}\}$.

The spin structures invariant to the groups of Examples 1) and 2) are illustrated in Figs. 1(a) and 2.

Until now we have considered G_{TSW} that contains all the elements of $\boldsymbol{P}$. In the cases of G_{TSW}'s involving only the elements of a subgroup $\boldsymbol{P}'$ of $\boldsymbol{P}$, it should be noted that any normal subgroup $\boldsymbol{N}(\subset \boldsymbol{P}')$ of $\boldsymbol{P}$ is a normal subgroup of $\boldsymbol{P}'$, but there may be other normal subgroups of $\boldsymbol{P}'$ which are not the normal subgroup of $\boldsymbol{P}$. However, all normal subgroups of $\boldsymbol{P}'$ are also found in Tables I and II. Then we can construct the group of TSW type in such a case without changing the above arguments.

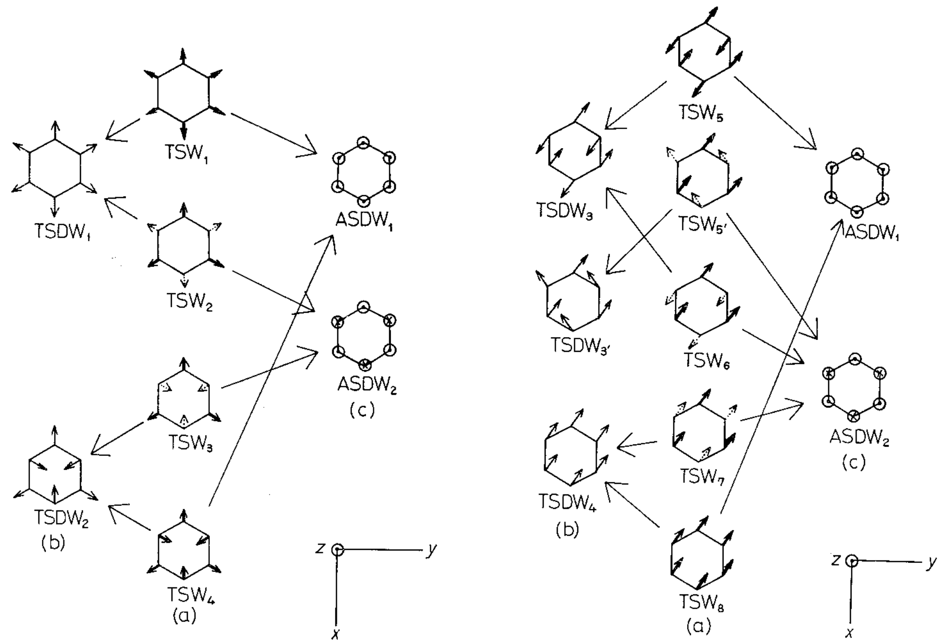

Fig. 1. The spin structures invariant to the groups in Example 1), (a), to those in Example 3), (b), and to those in Example 4), (c). The heavy and dotted arrows represent spin vectors inclined to the paper plane by an angle θ and $-\theta$ ($\theta \neq 0$ and $\pi/2$), respectively. The light arrows are in the paper plane. ⊙ and ⊗ are spin vectors vertical to the paper plane with up and down directions, respectively. $TSDW_3$ and $TSDW_4$ look like an ASDW when each vertex of the hexagon has only an electron, but when it has more than two electrons the directions of their spin vectors may be different in the paper plane.

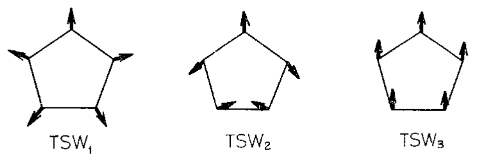

Fig. 2. The spin structures invariant to the groups in Example 2).

§ 4. Admissibility conditions of a subgroup to be the other types except TSW.

Now we consider subgroups of the other seven types in spin and time reversal symmetry except for TSW which were defined in II. Each subgroup of these types is obtained as a product group of a subgroup of TSW type ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{A})$ with one of the following seven subgroups $S\times T$, $M(\boldsymbol{e})$, T, $A(\boldsymbol{e})$, $A(\boldsymbol{e})M(\boldsymbol{e}')$ $(\boldsymbol{e}\boldsymbol{e}'=0)$, $A(\boldsymbol{e})\times T$, S and $S\times T$ where $M(\boldsymbol{e}) = \{E, tu(\boldsymbol{e}, \pi)\}$ and $A(\boldsymbol{e}) = \{u(\boldsymbol{e}, \theta), u(\boldsymbol{e}, \theta)\bar{E};$ $0 \leqq \theta \leqq 2\pi\}$. We denote any one of these groups by Γ. Not all of ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{A})$ form groups after multiplication by Γ. In order for the product ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{F}, \boldsymbol{A})\Gamma$ to be a group, the condition

$$ {}_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F},\boldsymbol{A})\,\Gamma=\Gamma\,{}_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F},\boldsymbol{A}) \tag{4·1}$$

must be satisfied. From this admissibility condition, it follows that

$$\bar{f}\Gamma=\Gamma\bar{f},\quad f\in\boldsymbol{F}. \tag{4·2}$$

Therefore, Γ is a normal subgroup of ${}_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F},\boldsymbol{A})\Gamma$. We call the $\boldsymbol{F}$'s satisfying this condition as the Γ admissible factor group. We denote the set of subgroups of TSW type with Γ admissible factor groups derived from P as $\mathscr{P}(\Gamma)$. Consider the following equivalence relation of the elements of $\mathscr{P}(\Gamma)$; for G_1 and G_2 in $\mathscr{P}(\Gamma)$, $G_1 \underset{\Gamma}{\sim} G_2$ if and only if $G_1\Gamma\sim G_2\Gamma$. Here it should be noted that even if $gG_1g^{-1}=G_2$ for $g\in G_0$, that is, $G_1\sim G_2$, it does not necessarily follow that $gG_1\Gamma g^{-1}=G_2\Gamma$, that is, $G_1\underset{\Gamma}{\sim}G_2$, because $gG_1\Gamma g^{-1}=gG_1g^{-1}g\Gamma g^{-1}=G_2g\Gamma g^{-1}\neq G_2\Gamma$ if $g\Gamma g^{-1}\neq\Gamma$. We call this equivalence the Γ-equivalence. We denote the Γ-equivalence class containing ${}_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F},\boldsymbol{A})$ as ${}_{II}\tilde{\boldsymbol{P}}^{\Gamma}(\boldsymbol{N},\boldsymbol{F},\boldsymbol{A})$. As a representative of a Γ-equivalence class, we shall choose ${}_{II}\boldsymbol{P}(\boldsymbol{N}_0,\boldsymbol{F}_0,\boldsymbol{A}_0)$ having a factor group with the minimum order, or a minimum factor group involving only proper rotations if the class contains factor groups of both proper and improper types as the minimum factor groups. We call this $\boldsymbol{F}_0$ as the representative factor group of the Γ-equivalence class. A subgroup of Γ type is specified by a representative factor group $\boldsymbol{F}_0$ and its automorphism $\boldsymbol{A}_0$.

Now, we shall obtain all the representative factor groups $\boldsymbol{F}_0$ of each Γ-equivalence class. In the following discussion, we put $\boldsymbol{e}=\boldsymbol{e}_z$ and $\boldsymbol{e}'=\boldsymbol{e}_y$ without loss of generality.

(1) TSW $(\Gamma={}_{II}\boldsymbol{C}_1)$

It is evident that any factor group is ${}_{II}\boldsymbol{C}_1$ admissible and a representative factor group.

(2) TSDW $(\Gamma=M(e_z))$

The admissibility condition is $\bar{f}tu(e_z,\pi)=\pm tu(e_z,\pi)\bar{f}$. Hence, $\bar{f}$ must be an element of ${}_{II}\boldsymbol{D}_\infty\times T$ and f belongs to $\boldsymbol{D}_\infty\times\boldsymbol{C}_I$. But, because it can be verified that for every $M(e_z)$ admissible $\boldsymbol{F}$ with improper rotations there is a unique proper point group $\boldsymbol{F}'$ and its automorphism $\boldsymbol{A}'$ such that ${}_{II}\boldsymbol{P}(\boldsymbol{N},\boldsymbol{F},\boldsymbol{A})M(e_z)\sim{}_{II}\boldsymbol{P}(\boldsymbol{N}',\boldsymbol{F}',\boldsymbol{A}')M(e_z)$, it is sufficient to consider only proper groups as the representative factor groups $\boldsymbol{F}_0$ of $M(e_z)$-equivalence classes. Then the admissibility condition is $\boldsymbol{F}_0\subseteq\boldsymbol{D}_\infty$. Now we consider which of the groups conjugate to $\boldsymbol{F}_0$ (including inner automorphisms of $\boldsymbol{F}_0$) can be a representative factor group of an $M(e_z)$-equivalence class. The conditions that a conjugate group $g\boldsymbol{F}_0g^{-1}$ of $\boldsymbol{F}_0$ by $g\in 0(3)$ is a representative factor group of an $M(e_z)$-equivalence class different from the one with $\boldsymbol{F}_0$ are $g\boldsymbol{F}_0g^{-1}\subseteq\boldsymbol{D}_\infty$ and $\bar{g}M(e_z)\bar{g}^{-1}\neq M(e_z)$. When $\boldsymbol{C}_n\subseteq\boldsymbol{F}_0$ $(n>3)$, $\bar{g}M(e_z)\bar{g}^{-1}=M(e_z)$ for all g such that $g\boldsymbol{F}_0g^{-1}\subseteq\boldsymbol{D}_\infty$. Then $g\boldsymbol{F}_0g^{-1}$ cannot be a representative factor group of an $M(e_z)$-equivalence class different from the one with $\boldsymbol{F}_0$.

Now we consider the exceptional cases $\boldsymbol{F}_0=\boldsymbol{C}_2$ and $\boldsymbol{F}_0=\boldsymbol{D}_2$.

a) $\boldsymbol{F}_0=\boldsymbol{C}_2$

In order that $g\boldsymbol{C}_2g^{-1}\subset\boldsymbol{D}_\infty$ and $gM(e_z)g^{-1}\neq M(e_z)$, g must be $\pi/2$ rotation around an axis perpendicular to e_z. We can choose e_y as this axis without loss of generality. Then $\boldsymbol{C}_2'=(E, C_{2x})$ is a representative factor group of an $M(e_z)$-equivalence class different from the one with $\boldsymbol{C}_2$.

b) $\boldsymbol{F}_0=\boldsymbol{D}_2$

In order that $g\boldsymbol{D}_2g^{-1}\subset\boldsymbol{D}_\infty$ and $gM(e_z)g^{-1}\neq M(e_z)$, g must be the element of $\boldsymbol{O}(3)$ such that $g\boldsymbol{D}_2g^{-1}=\boldsymbol{D}_2$, that is, $\boldsymbol{g}^\#\in\boldsymbol{I}(\boldsymbol{D}_2)$. It is easily found that there are just two subgroups ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{C}_3{}^{+\#})$ and ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{C}_3{}^{-\#})$ which are equivalent to and not $M(e_z)$-equivalent to ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{E})$. Because ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{C}_3{}^{+\#})M(e_z)\sim{}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{E})M(e_x)$ and ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{C}_3{}^{-\#})M(e_z)\sim{}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{E})M(e_y)$, we can take the products of ${}_{II}\boldsymbol{P}(\boldsymbol{N}, \boldsymbol{D}_2, \boldsymbol{E})$ with $M(e_z)$, $M(e_x)$ and $M(e_y)$ as the representatives of the subgroups of TSDW type with the factor group $\boldsymbol{D}_2$.

(3) TSCW ($\Gamma=T$)

It is evident that any factor group is T admissible and any T admissible factor group$\subseteq\boldsymbol{SO}(3)$ is the representative factor group of a T-equivalence class.

(4) ASW ($\Gamma=A(e_z)$)

From the admissibility condition $\bar{f}u(e_z, 0)=u(e_z, \theta')\bar{f}$, a factor group $\boldsymbol{F}$ is $A(e_z)$ admissible if and only if $\boldsymbol{F}\subset\boldsymbol{D}_\infty\times\boldsymbol{C}_I$. As $\bar{f}A(e_z)=EA(e_z)$ for any element $f\in\boldsymbol{F}$ contained in $\boldsymbol{C}_\infty$, the representative factor groups $\boldsymbol{F}_0$ of the $A(e_z)$-equivalence classes are the following: $\boldsymbol{C}_1$, $\boldsymbol{C}_I$, $\boldsymbol{C}_2'=(E, C_{2x})$, $\boldsymbol{C}_{1h}'=(E, IC_{2x})$ and $\boldsymbol{C}_{2h}'=(E, C_{2x})\times\boldsymbol{C}_I$ where the dash means that the axis of the C_2 rotation is e_x.

(5) ASDW ($\Gamma=A(e_z)M(e_y)$)

From the admissibility condition an $A(e_z)M(e_y)$ admissible factor group $\boldsymbol{F}$ must satisfy $\boldsymbol{F}\subseteq\boldsymbol{D}_\infty\times\boldsymbol{C}_I$. By an argument similar to the ones in the cases of TSDW and ASW, the representative factor groups of the $A(e_z)M(e_y)$-equivalence classes are $\boldsymbol{C}_1$ and $\boldsymbol{C}_2'$.

(6) ASCW ($\Gamma=A(e_z)\times T$)

The condition of $A(e_z)\times T$ admissible factor group $\boldsymbol{F}$ is $\boldsymbol{F}\subseteq\boldsymbol{D}_\infty\times\boldsymbol{C}_I$ and the representative factor groups of $A(e_z)\times T$-equivalence classes are $\boldsymbol{C}_1$ and $\boldsymbol{C}_2'$.

(7) CCW ($\Gamma=S$)

It is evident that all factor group are S admissible and there are only two S-equivalence classes with $\boldsymbol{C}_1$ and $\boldsymbol{C}_I$ as the representatives.

(8) TICS ($\Gamma=S\times T$)

It is evident that all factor groups are $S\times T$ admissible and $S\times T$ equivalent, so that there is only one $S\times T$-equivalence class with $\boldsymbol{C}_1$ as the representative.

We summarize in Table V the conditions on Γ admissible factor groups and the representative factor groups of Γ classes.

We give here, as an example, all subgroups of TSDW and ASDW types in the case $\boldsymbol{P}=\boldsymbol{C}_6$.

Table V. Γ admissible factor groups $\boldsymbol{F}$ and representative factor groups $\boldsymbol{F}_0$ of Γ-equivalence classes.

type	Γ	admissible factor group $\boldsymbol{F}$	representative factor group $\boldsymbol{F}_0$ of Γ class
TSW	${}_{II}\boldsymbol{C}_1$	$\boldsymbol{F}\subseteq\boldsymbol{O}(3)$	$\boldsymbol{F}_0\subseteq\boldsymbol{O}(3)$
TSDW	$M(e_z)$	$\boldsymbol{F}\subseteq\boldsymbol{D}_\infty\times\boldsymbol{C}_I$	$\boldsymbol{F}_0\subseteq\boldsymbol{D}_\infty$, $\boldsymbol{C}_2'=(E, C_{2x})$
	$M(e_z)$, $M(e_y)$	$\boldsymbol{F}\subseteq\boldsymbol{D}_2\times\boldsymbol{C}_I$	$\boldsymbol{D}_2$
TSCW	T	$\boldsymbol{F}\subseteq\boldsymbol{O}(3)$	$\boldsymbol{F}_0\subseteq\boldsymbol{SO}(3)$
ASW	$A(e_z)$	$\boldsymbol{F}\subseteq\boldsymbol{D}_\infty\times\boldsymbol{C}_I$	$\boldsymbol{C}_1, \boldsymbol{C}_I, \boldsymbol{C}_2'=(E, C_{2x})$, $\boldsymbol{C}_{1h}'=(E, IC_{2x})$ and $\boldsymbol{C}_{2h}'=(E, C_{2x})\times\boldsymbol{C}_I$
ASDW	$A(e_z)M(e_y)$	$\boldsymbol{F}\subseteq\boldsymbol{D}_\infty\times\boldsymbol{C}_I$	$\boldsymbol{C}_1$, $\boldsymbol{C}_2'$
ASCW	$A(e_z)\times T$	$\boldsymbol{F}\subseteq\boldsymbol{D}_\infty\times\boldsymbol{C}_I$	$\boldsymbol{C}_1$, $\boldsymbol{C}_2'$
CCW	S	$\boldsymbol{F}\subseteq\boldsymbol{O}(3)$	$\boldsymbol{C}_1$, $\boldsymbol{C}_I$
TICS	$S\times T$	$\boldsymbol{F}\subseteq\boldsymbol{O}(3)$	$\boldsymbol{C}_1$

Example 3) Subgroups of TSDW type in the case $\boldsymbol{P}=\boldsymbol{C}_6$.

The representative factor groups of $M(e_z)$-equivalence classes are $\boldsymbol{C}_6$, $\boldsymbol{C}_3$, $\boldsymbol{C}_2$, $\boldsymbol{C}_2'$ and $\boldsymbol{C}_1$, and the representatives of the subgroups of TSDW type are as follows:

$$G_{\mathrm{TSDW}_1}={}_{II}\boldsymbol{C}_6(\boldsymbol{C}_1, \boldsymbol{C}_6, \boldsymbol{E})M(e_z), \quad G_{\mathrm{TSDW}_2}={}_{II}\boldsymbol{C}_6(\boldsymbol{C}_2, \boldsymbol{C}_3, \boldsymbol{E})M(e_z),$$

$$G_{\mathrm{TSDW}_3}={}_{II}\boldsymbol{C}_6(\boldsymbol{C}_3, \boldsymbol{C}_2, \boldsymbol{E})M(e_z), \quad G_{\mathrm{TSDW}_{3'}}={}_{II}\boldsymbol{C}_6(\boldsymbol{C}_3, \boldsymbol{C}_2', \boldsymbol{E})M(e_z),$$

$$G_{\mathrm{TSDW}_4}={}_{II}\boldsymbol{C}_6(\boldsymbol{C}_6, \boldsymbol{C}_1, \boldsymbol{E})M(e_z).$$

The spin structures invariant to these groups are indicated in Fig. 1(b). It should be noted that G_{TSW_1} and G_{TSW_2} of Example 1) belong to ${}_{II}\tilde{\boldsymbol{C}}_6^{M(e_z)}(\boldsymbol{C}_1, \boldsymbol{C}_6, \boldsymbol{E})$, G_{TSW_3} and G_{TSW_4} to ${}_{II}\tilde{\boldsymbol{C}}_6^{M(e_z)}(\boldsymbol{C}_2, \boldsymbol{C}_3, \boldsymbol{E})$, G_{TSW_5} and G_{TSW_6} to ${}_{II}\tilde{\boldsymbol{C}}_6^{M(e_z)}(\boldsymbol{C}_3, \boldsymbol{C}_2, \boldsymbol{E})$, $G_{\mathrm{TSW}_{5'}}$ to ${}_{II}\tilde{\boldsymbol{C}}_6^{M(e_z)}(\boldsymbol{C}_3, \boldsymbol{C}_2', \boldsymbol{E})$ and G_{TSW_7} and G_{TSW_8} to ${}_{II}\tilde{\boldsymbol{C}}_6^{M(e_z)}(\boldsymbol{C}_6, \boldsymbol{C}_1, \boldsymbol{E})$. These relations are indicated by arrows in Fig. 1.

Example 4) Subgroups of ASDW type in the case $\boldsymbol{P}=\boldsymbol{C}_6$

The representative factor groups of $A(e_z)M(e_y)$-equivalence classes are $\boldsymbol{C}_1$ and $\boldsymbol{C}_2'$, and the representative subgroups of ASDW type are $G_{\mathrm{ASDW}_1}={}_{II}\boldsymbol{C}_6(\boldsymbol{C}_6, \boldsymbol{C}_1, \boldsymbol{E})A(e_z)M(e_y)$, $G_{\mathrm{ASDW}_2}={}_{II}\boldsymbol{C}_6(\boldsymbol{C}_3, \boldsymbol{C}_2', \boldsymbol{E})A(e_z)M(e_y)$. The spin structures invariant to these groups are indicated in Fig. 1(c). G_{TSW_1}, G_{TSW_4}, G_{TSW_5} and G_{TSW_8} belong to ${}_{II}\tilde{\boldsymbol{C}}_6^{A(e_z)M(e_y)}(\boldsymbol{C}_6, \boldsymbol{C}_1, \boldsymbol{E})$, G_{TSW_2}, G_{TSW_3}, $G_{\mathrm{TSW}_{5'}}$ G_{TSW_6} and G_{TSW_7} to ${}_{II}\tilde{\boldsymbol{C}}_6^{A(e_z)M(e_y)}(\boldsymbol{C}_3, \boldsymbol{C}_2', \boldsymbol{E})$. These relations are indicated by arrows in Fig. 1.

Until now we have considered only the case of the invariance group in which all the elements of $\boldsymbol{P}$ are contained. We can start from $\boldsymbol{P}'(\subset\boldsymbol{P})$ instead of $\boldsymbol{P}$ in a manner similar to the above discussion and construct the invariance groups. A solution of TICS type derived from $\boldsymbol{P}'$ is called a charge density wave (CDW) because it is not invariant to $p\notin\boldsymbol{P}'$ and has a charge density modulation at sites inequivalent with respect to $\boldsymbol{P}'$ (but equivalent with respect to $\boldsymbol{P}$). Solutions of the other types derived from $\boldsymbol{P}'$ also have a charge density modulation as well as a spin structure (TSW, TSDW, ASW, ASDW, and ASCW) or a charge current structure (CCW).

Appendix 1

——Proof of Theorem 1——

We first show that $\boldsymbol{Z}(\boldsymbol{F})$ is a normal subgroup of $\boldsymbol{H}(\boldsymbol{F})$. Let us decompose $\boldsymbol{H}(\boldsymbol{F})$ into the right cosets with respect to $\boldsymbol{Z}(\boldsymbol{F})$; $\boldsymbol{H}(\boldsymbol{F})=\{\boldsymbol{Z}(\boldsymbol{F})a_p\}$. For any $y, z\in\boldsymbol{Z}(\boldsymbol{F})$, $a_p\in\boldsymbol{H}(\boldsymbol{F})$ and $f\in\boldsymbol{F}$, we have $[(ya_p)^{-1}z(ya_p)]^{-1}f(ya_p)^{-1}zya_p=a_p^{-1}(y^{-1}zy)^{-1}f'(y^{-1}zy)a_p=a_p^{-1}f'a_p=f$ where $f'=a_pfa_p^{-1}\in\boldsymbol{F}$, so that $(ya_p)^{-1}zya_p\in\boldsymbol{Z}(\boldsymbol{F})$, that is, $\boldsymbol{Z}(\boldsymbol{F})$ is a normal subgroup of $\boldsymbol{H}(\boldsymbol{F})$. Next we show that all elements of a coset $\boldsymbol{Z}(\boldsymbol{F})a_p$ give a same automorphism of $\boldsymbol{F}$. The inner automorphism by z_ia_p, where $z_i\in\boldsymbol{Z}(\boldsymbol{F})$, is $(z_ia_p)^{-1}f(z_ia_p)=a_p^{-1}fa_p$. Furthermore, we can see that the elements of different cosets of $\boldsymbol{Z}(\boldsymbol{F})$ give different inner automorphisms; if $g_1^{-1}fg_1=g_2^{-1}fg_2$ for any $f\in\boldsymbol{F}$, then $(g_1g_2^{-1})^{-1}f(g_1g_2^{-1})=f$, that is, $g_1g_2^{-1}\in\boldsymbol{Z}(\boldsymbol{F})$. Therefore, g_1 and g_2 are in a same coset of $\boldsymbol{Z}(\boldsymbol{F})$. Hence, we see that there is a one to one correspondence between $\boldsymbol{H}(\boldsymbol{F})/\boldsymbol{Z}(\boldsymbol{F})$ and inner automorphisms of $\boldsymbol{F}$.

Appendix 2

——Proof of Theorem 2——

Let us denote the elements of a coset $\boldsymbol{I}(\boldsymbol{F})\mathbf{t}_\alpha$ by $\mathbf{w}_i{}^\#\mathbf{t}_\alpha$, where $\mathbf{w}_i{}^\#$ is the inner automorphism by $\mathbf{w}_i\in\boldsymbol{H}(\boldsymbol{F})$. Then for any $f\in\boldsymbol{F}$, $(\mathbf{w}_2{}^\#\mathbf{t}_\alpha)(f)=W_2^{-1}(\mathbf{t}_\alpha(f))w_2=(w_1^{-1}w_2)^{-1}w_1^{-1}(\mathbf{t}_\alpha(f))w_1(w_1^{-1}w_2)$. That is, $(\mathbf{w}_2{}^\#\mathbf{t}_\alpha)(f)$ is conjugate to $(\mathbf{w}_1{}^\#\mathbf{t}_\alpha)(f)$ (for any $w_1\in\boldsymbol{H}(\boldsymbol{F})$) by $(w_1^{-1}w_2)\in\boldsymbol{H}(\boldsymbol{F})$. Inversely for any pair of automorphisms $\mathbf{c}$ and $\mathbf{d}$ which can be transferred by a conjugation, $\mathbf{c}(f)=s^{-1}(\mathbf{d}(f))s=(\mathbf{s}^\#\mathbf{d})(f)$ for some $s\in\boldsymbol{H}(\boldsymbol{F})$. Then $\mathbf{c}$ and $\mathbf{d}$ are in a same right coset. This completes the proof of the theorem.

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