# Classification of the possible symmetries of the Jahn—Teller systems

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On the basis of group-theoretical approach we elaborated the complete classification of possible symmetries of extremal points of potential energy surfaces of Jahn—Teller systems for all symmetry point groups. The method originates from the principle of step-by-step splitting of degenerate irreducible representations of corresponding electron terms due to the lowering of the symmetry of the system. It was shown that the existence of some deformations cannot be the result of the Jahn—Teller effect contrary to the fact that also such an explanation is at present used.

На основе группово-теоретического подхода мы разработали полную классификацию возможных симметрий экстремальных точек поверхностей потенциальной энергии систем Яна—Теллера для всех точечных групп симметрии. Этот метод проистекает из принципа постадийного расщепления вырожденных неприводимых представлений соответствующих электронных термов вследствие понижения симметрии системы. Было показано, что существование некоторых искажений не может являться следствием эффекта Яна—Теллера, вопреки тому, что подобное объяснение также используется в настоящее время.

The problem of symmetry of systems which originate through Jahn—Teller deformation from the original highly symmetrical system, was mostly solved by analytical methods of searching for extrema of adiabatic potential surface [1—15]. Such an attempt to solve this problem has two major disadvantages:

i) Analytical forms of adiabatic potential surfaces are determined by perturbation theory, using the Taylor expansion of vibronic Hamiltonian. The number of extrema from such adiabatic potential surfaces is then dependent on the order of perturbation theory used as well as on the number of terms in the Taylor expansion of vibronic Hamiltonian.

ii) The problem of obtaining the extremal points from adiabatic potential of more complex forms is transformed to the problem of solving the system of nonlinear equations. We note that there does not exist any algorithm which guaranties obtaining all the extremal points.

Some authors [16—19] used the group-theoretical approach to solve this problem using the symmetry of the Jahn—Teller active coordinates. Even this approach did not give the complete solution of the problem, because the obtained results satisfy only the first order of perturbation theory.

In our work we present the complete group-theoretical analysis of symmetries of the Jahn—Teller systems of all molecular symmetry point groups.

## Method and results

The Jahn—Teller effect may appear only in the nonlinear systems with such a symmetry group which possesses at least one multi-dimensional irreducible representation. Mostly this is two-dimensional degenerate $E$-representation and/or three-times degenerate $T$-representation. In the case of symmetry groups $I_h$ and $I$ yet four-times degenerate $G$-representation and five-times degenerate $H$-representation appear. Such a multi-dimensional representation splits due to the Jahn—Teller effect into the representation of lower order (until the nondegenerate representation is achieved) lowering the symmetry of the system. Therefore the problem to determine the extremal points of the Jahn—Teller systems is thus reduced to find all the symmetry point groups which satisfy the following conditions:

i) They are the subgroups of original symmetry group of the system in which the Jahn—Teller effect appears.

ii) By splitting the degenerate irreducible representations there appears at least one nondegenerate irreducible representation.

iii) The subgroups are not permitted if there exists the transition group (such that it causes the step-by-step lowering of symmetry of original group to the final subgroup) while the degeneracy is removed already in the transition group.

For our purposes still further division of such subgroups into some levels will be useful. In the first level there are groups which are the subgroups of the former original symmetry group of studied system and are not the subgroups of any other subgroups. In the second level there will be groups which are the subgroups of the original group as well as of the groups from the first level. In the third level there will be groups which are the subgroups of the original group as well as of the groups from the first and the second level, *etc.* The order of the original symmetry group is the integer multiple of the orders of its subgroups [20, 21]. This gives us the number of equivalent geometries of extremal points of adiabatic potential surface, which correspond to the system with the symmetry of the given subgroup.

The hierarchy of molecular symmetry point groups as well as their subgroups is presented in Fig. 1. The common dihedral and cyclic groups have been arranged in the figure in descending sequence from groups of the highest to the lowest order. This enables all the subgroups of a particular point group to be noted at a glance. The quotient of the order of given group and its subgroups must be a small integer greater than unity. The icosahedral

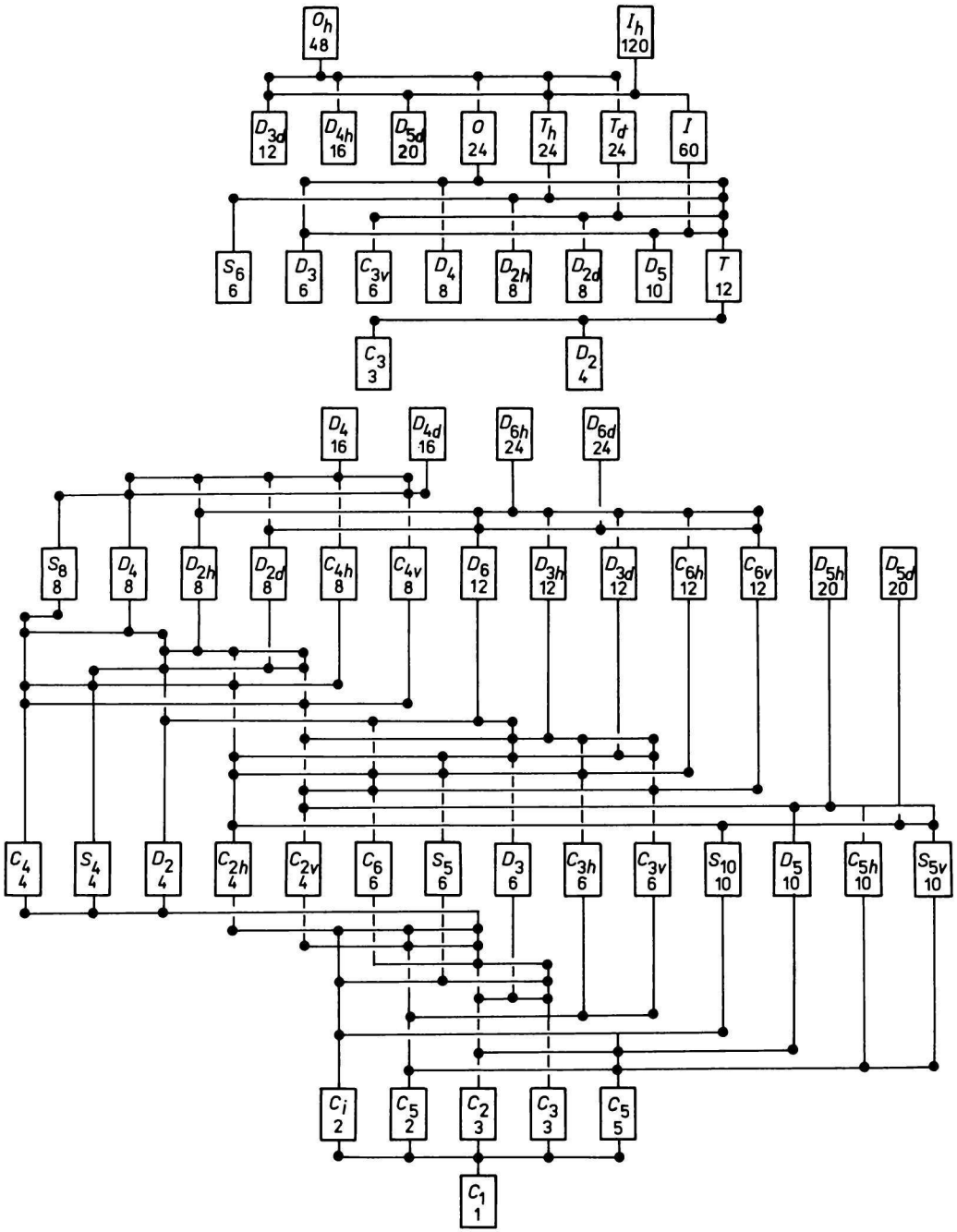


*Fig. 1.* Hierarchy of molecular symmetry point groups.

and cubic groups have been arranged in a similar figure and the descent in symmetry continued until correspondence with the other part of figure was achieved.

The results of group-theoretical analysis of all the symmetry point groups (containing the degenerate irreducible representations) of molecules are presented in Table 1. Subgroups fulfilling the three mentioned conditions are ordered into individual levels. For each subgroup we also present the irreducible representations to which the stable electron term can be ascribed.

*Table 1*

Possible symmetries of the extremal points of Jahn—Teller systems[a]

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| $O_h$ | 48 | $E_g$ | 1 | $D_{4h}$ | 16 | 3 | $A_{1g}$, $B_{1g}$ |
| | | | 2 | $D_4$ | 8 | 6 | $A_1$, $B_1$ |
| | | | | $D_{2h}$ | 8 | 6 | $A_g$ |
| | | | | $D_{2d}$ | 8 | 6 | $A_1$, $B_1$ |
| | | | | $C_{2h}$ | 4 | 12 | $A_g$, $B_g$ |
| | | | 3 | $D_2$ | 4 | 12 | $A$ |
| | | | | $C_2$ | 2 | 24 | $A$, $B$ |
| | | | | $C_i$ | 2 | 24 | $A_g$ |
| | | | | $C_s$ | 2 | 24 | $A'$, $A''$ |
| | | $E_u$ | 1 | $D_{4h}$ | 16 | 3 | $A_{1u}$, $B_{1u}$ |
| | | | 2 | $D_4$ | 8 | 6 | $A_1$, $B_1$ |
| | | | | $D_{2h}$ | 8 | 6 | $A_u$ |
| | | | | $D_{2d}$ | 8 | 6 | $A_1$, $B_1$ |
| | | | | $C_{2h}$ | 4 | 12 | $A_u$, $B_u$ |
| | | | 3 | $D_2$ | 4 | 12 | $A$ |
| | | | | $C_2$ | 2 | 24 | $A$, $B$ |
| | | | | $C_i$ | 2 | 24 | $A_u$ |
| | | | | $C_s$ | 2 | 24 | $A'$, $A''$ |
| | | $T_{1g}$ | 1 | $D_{4h}$ | 16 | 3 | $A_{2g}$ |
| | | | | $D_{3d}$ | 12 | 4 | $A_{2g}$ |
| | | | 2 | $D_4$ | 8 | 6 | $A_2$ |
| | | | | $D_3$ | 6 | 8 | $A_2$ |
| | | | | $D_{2d}$ | 8 | 6 | $A_2$ |
| | | | | $D_{2h}$ | 8 | 6 | $B_{1g}$, $B_{2g}$, $B_{3g}$ |
| | | | | $S_6$ | 6 | 8 | $A_g$ |
| | | | | $C_{3v}$ | 6 | 8 | $A_2$ |
| | | | | $C_{2h}$ | 4 | 12 | $A_g$, $B_g$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | | 3 | $D_2$ | 4 | 12 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 16 | $A$ |
| | | | | $C_{2v}$ | 4 | 12 | $B_1$, $B_2$ |
| | | | | $C_{2h}$ | 4 | 12 | $B_g$ |
| | | | | $C_2$ | 2 | 24 | $A$, $B$ |
| | | | | $C_i$ | 2 | 24 | $A_g$ |
| | | | | $C_s$ | 2 | 24 | $A'$, $A''$ |
| | | | 4 | $C_2$ | 2 | 24 | $B$ |
| | | $T_{2g}$ | 1 | $D_{4h}$ | 16 | 3 | $B_{2g}$ |
| | | | | $D_{3d}$ | 12 | 4 | $A_{1g}$ |
| | | | 2 | $D_4$ | 8 | 6 | $B_2$ |
| | | | | $D_3$ | 6 | 8 | $A_1$ |
| | | | | $D_{2d}$ | 8 | 6 | $B_2$ |
| | | | | $D_{2h}$ | 8 | 6 | $B_{1g}$, $B_{2g}$, $B_{3g}$ |
| | | | | $S_6$ | 6 | 8 | $A_g$ |
| | | | | $C_{3v}$ | 6 | 8 | $A_1$ |
| | | | | $C_{2h}$ | 4 | 12 | $A_g$, $B_g$ |
| | | | 3 | $D_2$ | 4 | 12 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 16 | $A$ |
| | | | | $C_{2v}$ | 4 | 12 | $B_1$, $B_2$ |
| | | | | $C_{2h}$ | 4 | 12 | $B_g$ |
| | | | | $C_2$ | 2 | 24 | $A$, $B$ |
| | | | | $C_i$ | 2 | 24 | $A_g$ |
| | | | | $C_s$ | 2 | 24 | $A'$, $A''$ |
| | | | 4 | $C_2$ | 2 | 24 | $B$ |
| | | $T_{1u}$ | 1 | $D_{4h}$ | 16 | 3 | $A_{2u}$ |
| | | | | $D_{3d}$ | 12 | 4 | $A_{2u}$ |
| | | | 2 | $D_4$ | 8 | 6 | $A_2$ |
| | | | | $D_3$ | 6 | 8 | $A_2$ |
| | | | | $D_{2d}$ | 8 | 6 | $B_2$ |
| | | | | $D_{2h}$ | 8 | 6 | $B_{1u}$, $B_{2u}$, $B_{3u}$ |
| | | | | $S_6$ | 6 | 8 | $A_u$ |
| | | | | $C_{3v}$ | 6 | 8 | $A_1$ |
| | | | | $C_{2h}$ | 4 | 12 | $A_u$, $B_u$ |
| | | | 3 | $D_2$ | 4 | 12 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 16 | $A$ |
| | | | | $C_{2v}$ | 4 | 12 | $B_1$, $B_2$ |
| | | | | $C_{2h}$ | 4 | 12 | $B_u$ |
| | | | | $C_2$ | 2 | 24 | $A$, $B$ |
| | | | | $C_i$ | 2 | 24 | $A_u$ |
| | | | | $C_s$ | 2 | 24 | $A'$, $A''$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | | 4 | $C_2$ | 2 | 24 | $B$ |
| | | $T_{2u}$ | 1 | $D_{4h}$ | 16 | 3 | $B_{2u}$ |
| | | | | $D_{3d}$ | 12 | 4 | $A_{1u}$ |
| | | | 2 | $D_4$ | 8 | 6 | $B_2$ |
| | | | | $D_3$ | 6 | 8 | $A_1$ |
| | | | | $D_{2d}$ | 8 | 6 | $B_2$ |
| | | | | $D_{2h}$ | 8 | 6 | $B_{1u}$, $B_{2u}$, $B_{3u}$ |
| | | | | $S_6$ | 6 | 8 | $A_u$ |
| | | | | $C_{3v}$ | 6 | 8 | $A_2$ |
| | | | | $C_{2h}$ | 4 | 12 | $A_u$, $B_u$ |
| | | | 3 | $D_2$ | 4 | 12 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 16 | $A$ |
| | | | | $C_{2v}$ | 4 | 12 | $B_1$, $B_2$ |
| | | | | $C_{2h}$ | 4 | 12 | $B_u$ |
| | | | | $C_2$ | 2 | 24 | $A$, $B$ |
| | | | | $C_i$ | 2 | 24 | $A_u$ |
| | | | | $C_s$ | 2 | 24 | $A'$, $A''$ |
| | | | 4 | $C_2$ | 2 | 24 | $B$ |
| $I_h$ | 120 | $T_{1g}$ | 1 | $D_{5d}$ | 20 | 6 | $A_{2g}$ |
| | | | | $D_{3d}$ | 12 | 10 | $A_{2g}$ |
| | | | 2 | $D_5$ | 10 | 12 | $A_2$ |
| | | | | $D_3$ | 6 | 20 | $A_2$ |
| | | | | $D_{2h}$ | 8 | 15 | $B_{1g}$, $B_{2g}$, $B_{3g}$ |
| | | | | $S_6$ | 6 | 20 | $A_g$ |
| | | | | $C_{2h}$ | 4 | 30 | $A_g$, $B_g$ |
| | | | 3 | $D_2$ | 4 | 30 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 40 | $A$ |
| | | | | $C_2$ | 2 | 60 | $A$, $B$ |
| | | | | $C_i$ | 2 | 60 | $A_g$ |
| | | | | $C_s$ | 2 | 60 | $A'$, $A''$ |
| | | $T_{1u}$ | 1 | $D_{5d}$ | 20 | 6 | $A_{2u}$ |
| | | | | $D_{3d}$ | 12 | 10 | $A_{2u}$ |
| | | | 2 | $D_5$ | 10 | 12 | $A_2$ |
| | | | | $D_3$ | 6 | 20 | $A_2$ |
| | | | | $D_{2h}$ | 8 | 15 | $B_{1u}$, $B_{2u}$, $B_{3u}$ |
| | | | | $S_6$ | 6 | 20 | $A_u$ |
| | | | | $C_{2h}$ | 4 | 30 | $A_u$, $B_u$ |
| | | | 3 | $D_2$ | 3 | 40 | $A$ |
| | | | | $C_2$ | 2 | 60 | $A$, $B$ |
| | | | | $C_i$ | 2 | 60 | $A_u$ |
| | | | | $C_s$ | 2 | 60 | $A'$, $A''$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | $G_g$ | 1 | $T_h$ | 24 | 5 | $A_g$ |
| | | | | $D_{3d}$ | 12 | 10 | $A_{1g}$, $A_2$ |
| | | | 2 | $T$ | 12 | 10 | $A$ |
| | | | | $D_3$ | 6 | 20 | $A_1$, $A_2$ |
| | | | | $D_{2h}$ | 8 | 15 | $B_{1g}$, $B_{2g}$, $B_{3g}$ |
| | | | | $S_6$ | 6 | 20 | $A_g$ |
| | | | | $C_{2h}$ | 4 | 30 | $A_g$, $B_g$ |
| | | | 3 | $D_2$ | 4 | 30 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 40 | $A$ |
| | | | | $C_2$ | 2 | 60 | $A$, $B$ |
| | | | | $C_i$ | 2 | 60 | $A_g$ |
| | | | | $C_s$ | 2 | 60 | $A'$, $A''$ |
| | | $G_u$ | 1 | $T_h$ | 24 | 5 | $A_u$ |
| | | | | $D_{3d}$ | 12 | 10 | $A_{1u}$, $A_{2u}$ |
| | | | 2 | $T$ | 12 | 10 | $A$ |
| | | | | $D_3$ | 6 | 20 | $A_1$, $A_2$ |
| | | | | $D_{2h}$ | 8 | 15 | $B_{1u}$, $B_{2u}$, $B_{3u}$ |
| | | | | $S_6$ | 6 | 20 | $A_u$ |
| | | | | $C_{2h}$ | 4 | 30 | $A_u$, $B_u$ |
| | | | | $D_2$ | 4 | 30 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 40 | $A$ |
| | | | | $C_2$ | 2 | 60 | $A$, $B$ |
| | | | | $C_i$ | 2 | 60 | $A_u$ |
| | | | | $C_s$ | 2 | 60 | $A'$, $A''$ |
| | | $H_g$ | 1 | $D_{5d}$ | 20 | 6 | $A_{1g}$ |
| | | | | $D_{3d}$ | 12 | 10 | $A_{1g}$ |
| | | | 2 | $D_5$ | 10 | 12 | $A_1$ |
| | | | | $D_3$ | 6 | 20 | $A_1$ |
| | | | | $D_{2h}$ | 8 | 15 | $A_g$, $B_{1g}$, $B_{2g}$, $B_{3g}$ |
| | | | | $S_6$ | 6 | 20 | $A_g$ |
| | | | | $C_{2h}$ | 4 | 30 | $A_g$, $B_g$ |
| | | | 3 | $D_2$ | 4 | 30 | $A$, $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 40 | $A$ |
| | | | | $C_2$ | 2 | 60 | $A$, $B$ |
| | | | | $C_i$ | 2 | 60 | $A_g$ |
| | | | | $C_s$ | 2 | 60 | $A'$, $A''$ |
| | | $H_u$ | 1 | $D_{5d}$ | 20 | 6 | $A_{1u}$ |
| | | | | $D_{3d}$ | 12 | 10 | $A_{1u}$ |
| | | | 2 | $D_5$ | 10 | 12 | $A_1$ |
| | | | | $D_3$ | 6 | 20 | $A_1$ |
| | | | | $D_{2h}$ | 8 | 15 | $A_u$, $B_{1u}$, $B_{2u}$, $B_{3u}$ |
| | | | | $S_6$ | 6 | 20 | $A_u$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | | | $C_{2h}$ | 4 | 30 | $A_u$, $B_u$ |
| | | | 3 | $D_2$ | 4 | 30 | $A$, $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 40 | $A$ |
| | | | | $C_2$ | 2 | 60 | $A$, $B$ |
| | | | | $C_i$ | 2 | 60 | $A_u$ |
| | | | | $C_s$ | 2 | 60 | $A'$, $A''$ |
| $T_d$ | 24 | $E$ | 1 | $D_{2d}$ | 8 | 3 | $A_1$, $B_1$ |
| | | | 2 | $D_2$ | 4 | 6 | $A$ |
| | | | | $C_s$ | 2 | 12 | $A'$, $A''$ |
| | | $T_1$ | 1 | $D_{2d}$ | 8 | 3 | $A_2$ |
| | | | | $C_{3v}$ | 6 | 4 | $A_2$ |
| | | | 2 | $D_2$ | 4 | 6 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 8 | $A$ |
| | | | | $C_{2v}$ | 4 | 6 | $B_1$, $B_2$ |
| | | | | $C_2$ | 2 | 12 | $B$ |
| | | | | $C_s$ | 2 | 12 | $A'$, $A''$ |
| | | $T_2$ | 1 | $D_{2d}$ | 8 | 3 | $B_2$ |
| | | | | $C_{3v}$ | 6 | 4 | $A_1$ |
| | | | 2 | $D_2$ | 4 | 6 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 8 | $A$ |
| | | | | $C_{2v}$ | 4 | 6 | $B_1$, $B_2$ |
| | | | | $C_2$ | 2 | 12 | $B$ |
| | | | | $C_s$ | 2 | 12 | $A'$, $A''$ |
| $T_h$ | 24 | $E_g$ | 1 | $D_{2h}$ | 8 | 3 | $A_g$ |
| | | | 2 | $D_2$ | 4 | 6 | $A$ |
| | | | | $C_i$ | 2 | 12 | $A_g$ |
| | | $E_u$ | 1 | $D_{2h}$ | 8 | 3 | $A_u$ |
| | | | 2 | $D_2$ | 4 | 6 | $A$ |
| | | | | $C_i$ | 2 | 12 | $A_u$ |
| | | $T_g$ | 1 | $D_{2h}$ | 8 | 3 | $B_{1g}$, $B_{2g}$, $B_{3g}$ |
| | | | | $S_6$ | 6 | 4 | $A_g$ |
| | | | 2 | $D_2$ | 3 | 8 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 8 | $A$ |
| | | | | $C_i$ | 2 | 12 | $A_g$ |
| | | $T_u$ | 1 | $D_{2h}$ | 8 | 3 | $B_{1u}$, $B_{2u}$, $B_{3u}$ |
| | | | | $S_6$ | 6 | 4 | $A_u$ |
| | | | 2 | $D_2$ | 4 | 6 | $B_1$, $B_2$, $B_3$ |
| | | | | $C_3$ | 3 | 8 | $A$ |
| | | | | $C_i$ | 2 | 12 | $A_u$ |
| $O$ | 24 | $E$ | 1 | $D_4$ | 8 | 3 | $A_1$, $B_1$ |
| | | | 2 | $D_2$ | 4 | 6 | $A$ |
| | | | | $C_2$ | 2 | 12 | $A$, $B$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | $T_1$ | 1 | $D_4$ | 8 | 3 | $A_2$ |
| | | | | $D_3$ | 6 | 4 | $A_2$ |
| | | | 2 | $D_2$ | 4 | 6 | $B_1, B_2, B_3$ |
| | | | | $C_3$ | 3 | 8 | $A$ |
| | | | | $C_2$ | 2 | 12 | $A, B$ |
| | | $T_2$ | 1 | $D_4$ | 8 | 3 | $B_2$ |
| | | | | $D_3$ | 6 | 4 | $A_1$ |
| | | | 2 | $D_2$ | 4 | 6 | $B_1, B_2, B_3$ |
| | | | | $C_3$ | 3 | 8 | $A$ |
| | | | | $C_2$ | 2 | 12 | $A, B$ |
| $I$ | 60 | $T_1$ | 1 | $D_5$ | 10 | 6 | $A_2$ |
| | | | | $D_3$ | 6 | 10 | $A_2$ |
| | | | 2 | $D_2$ | 4 | 15 | $B_1, B_2, B_3$ |
| | | | | $C_3$ | 3 | 20 | $A$ |
| | | | | $C_2$ | 2 | 30 | $A, B$ |
| | | $T_2$ | 1 | $D_5$ | 10 | 6 | $A_2$ |
| | | | | $D_3$ | 6 | 10 | $A_2$ |
| | | | 2 | $D_2$ | 4 | 15 | $B_1, B_2, B_3$ |
| | | | | $C_3$ | 3 | 20 | $A$ |
| | | | | $C_2$ | 2 | 30 | $A, B$ |
| | | $G$ | 1 | $T$ | 12 | 5 | $A$ |
| | | | | $D_3$ | 6 | 10 | $A_1, A_2$ |
| | | | 2 | $D_2$ | 4 | 15 | $B_1, B_2, B_3$ |
| | | | | $C_3$ | 3 | 20 | $A$ |
| | | | | $C_2$ | 2 | 30 | $A, B$ |
| | | $H$ | 1 | $D_5$ | 10 | 6 | $A_1$ |
| | | | | $D_3$ | 6 | 10 | $A_1$ |
| | | | 2 | $D_2$ | 4 | 15 | $A, B_1, B_2, B_3$ |
| | | | | $C_3$ | 3 | 20 | $A$ |
| | | | | $C_2$ | 2 | 30 | $A, B$ |
| $T$ | 12 | $E$ | 1 | $D_2$ | 4 | 3 | $A$ |
| | | $T$ | 1 | $D_2$ | 4 | 3 | $B_1, B_2, B_3$ |
| | | | | $C_3$ | 3 | 4 | $A$ |
| $D_{6h}$ | 24 | $E_{1g}$ | 1 | $D_{2h}$ | 8 | 3 | $B_{2g}, B_{3g}$ |
| | | | 2 | $D_2$ | 4 | 6 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 6 | $A_2, B_1, B_2$ |
| | | | | $C_{2h}$ | 4 | 6 | $A_g, B_g$ |
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_i$ | 2 | 12 | $A_g$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| | | $E_{2g}$ | 1 | $D_{2h}$ | 8 | 3 | $A_g, B_{1g}$ |
| | | | 2 | $D_2$ | 4 | 6 | $A, B_1$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | | | $C_{2v}$ | 4 | 6 | $A_1, A_2, B_2$ |
| | | | | $C_{2h}$ | 4 | 6 | $A_g, B_g$ |
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_i$ | 2 | 12 | $A_g$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| | | $E_{1u}$ | 1 | $D_{2h}$ | 8 | 3 | $B_{2u}, B_{3u}$ |
| | | | 2 | $D_2$ | 4 | 6 | $A, B_1$ |
| | | | | $C_{2v}$ | 4 | 6 | $A_1, B_1, B_2$ |
| | | | | $C_{2h}$ | 4 | 6 | $A_u, B_u$ |
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_i$ | 2 | 12 | $A_u$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| | | $E_{2u}$ | 1 | $D_{2h}$ | 8 | 3 | $A_u, B_{1u}$ |
| | | | 2 | $D_2$ | 4 | 6 | $A, B_1$ |
| | | | | $C_{2v}$ | 4 | 6 | $A_1, A_2, B_1$ |
| | | | | $C_{2h}$ | 4 | 6 | $A_u, B_u$ |
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_i$ | 2 | 12 | $A_u$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| $D_{6d}$ | 24 | $E_1$ | 2 | $D_2$ | 4 | 6 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 6 | $B_1, B_2$ |
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| | | $E_2$ | 1 | $D_{2d}$ | 8 | 3 | $B_1, B_2$ |
| | | | 2 | $D_2$ | 4 | 6 | $A, B_1$ |
| | | | | $C_{2v}$ | 4 | 6 | $A_1, A_2$ |
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| | | $E_3$ | 1 | $D_6$ | 12 | 2 | $B_1, B_2$ |
| | | | | $C_{6v}$ | 12 | 2 | $B_1, B_2$ |
| | | | 2 | $D_2$ | 4 | 6 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 6 | $B_1, B_2$ |
| | | | 3 | $C_2$ | 2 | 12 | $B$ |
| | | $E_4$ | 1 | $D_{2d}$ | 8 | 3 | $A_1, A_2$ |
| | | | 2 | $D_2$ | 4 | 6 | $A, B_1$ |
| | | | | $C_{2v}$ | 4 | 6 | $A_1, B_2$ |
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| | | $E_5$ | 2 | $D_2$ | 4 | 6 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 6 | $B_1, B_2$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | | 3 | $C_2$ | 2 | 12 | $A, B$ |
| | | | | $C_s$ | 2 | 12 | $A', A''$ |
| $D_6$ | 12 | $E_1$ | 1 | $D_2$ | 4 | 3 | $B_2, B_3$ |
| | | | 2 | $C_2$ | 2 | 6 | $A, B$ |
| | | $E_2$ | 1 | $D_2$ | 4 | 3 | $A, B_1$ |
| | | | 2 | $C_2$ | 2 | 6 | $A, B$ |
| $D_{5h}$ | 20 | $E_1'$ | 1 | $C_{2v}$ | 4 | 5 | $A_1, B_1$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| | | $E_2'$ | 1 | $C_{2v}$ | 4 | 5 | $A_1, B_1$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| | | $E_1''$ | 1 | $C_{2v}$ | 4 | 5 | $A_2, B_2$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| | | $E_2''$ | 1 | $C_{2v}$ | 4 | 5 | $A_2, B_2$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| $D_{5d}$ | 20 | $E_{1g}$ | 1 | $C_{2h}$ | 4 | 5 | $A_g, B_g$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_i$ | 2 | 10 | $A_g$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| | | $E_{2g}$ | 1 | $C_{2h}$ | 4 | 5 | $A_g, B_g$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_i$ | 2 | 10 | $A_g$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| | | $E_{1u}$ | 1 | $C_{2h}$ | 4 | 5 | $A_u, B_u$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_i$ | 2 | 10 | $A_u$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| | | $E_{2u}$ | 1 | $C_{2h}$ | 4 | 5 | $A_u, B_u$ |
| | | | 2 | $C_2$ | 2 | 10 | $A, B$ |
| | | | | $C_i$ | 2 | 10 | $A_u$ |
| | | | | $C_s$ | 2 | 10 | $A', A''$ |
| $D_5$ | 10 | $E_1$ | 1 | $C_2$ | 2 | 5 | $A, B$ |
| | | $E_2$ | 1 | $C_2$ | 2 | 5 | $A, B$ |
| $D_{4h}$ | 16 | $E_g$ | 1 | $D_{2h}$ | 8 | 2 | $B_{2g}, B_{3g}$ |
| | | | 2 | $D_2$ | 4 | 4 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 4 | $B_1, B_2$ |
| | | | | $C_{2h}$ | 4 | 4 | $B_g$ |
| | | | 3 | $C_2$ | 2 | 8 | $B$ |
| | | $E_u$ | 1 | $D_{2h}$ | 8 | 2 | $B_{2u}, B_{3u}$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | | 2 | $D_2$ | 4 | 4 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 4 | $B_1, B_2$ |
| | | | | $C_{2h}$ | 4 | 4 | $B_u$ |
| | | | 3 | $C_2$ | 2 | 8 | $B$ |
| $D_{4d}$ | 16 | $E_1$ | 2 | $D_2$ | 4 | 4 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 4 | $B_1, B_2$ |
| | | | 3 | $C_2$ | 2 | 8 | $B$ |
| | | $E_2$ | 1 | $D_4$ | 8 | 2 | $B_1, B_2$ |
| | | | | $C_{4v}$ | 8 | 2 | $B_1, B_2$ |
| | | | 2 | $C_4$ | 4 | 4 | $B$ |
| | | $E_3$ | 2 | $D_2$ | 4 | 4 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 4 | $B_1, B_2$ |
| | | | 3 | $C_2$ | 2 | 8 | $B$ |
| $D_4$ | 8 | $E$ | 1 | $D_2$ | 4 | 2 | $B_2, B_3$ |
| | | | 2 | $C_2$ | 2 | 4 | $B$ |
| $D_{3h}$ | 12 | $E'$ | 1 | $C_{2v}$ | 4 | 3 | $A_1, B_2$ |
| | | | 2 | $C_2$ | 2 | 6 | $A, B$ |
| | | | | $C_s$ | 2 | 6 | $A', A''$ |
| | | $E''$ | 1 | $C_{2v}$ | 4 | 3 | $A_2, B_1$ |
| | | | 2 | $C_2$ | 2 | 6 | $A, B$ |
| | | | | $C_s$ | 2 | 6 | $A', A''$ |
| $D_{3d}$ | 12 | $E_g$ | 1 | $C_{2h}$ | 4 | 3 | $A_g, B_g$ |
| | | | 2 | $C_2$ | 2 | 6 | $A, B$ |
| | | | | $C_i$ | 2 | 6 | $A_g$ |
| | | | | $C_s$ | 2 | 6 | $A', A''$ |
| | | $E_u$ | 1 | $C_{2h}$ | 4 | 3 | $A_u, B_u$ |
| | | | 2 | $C_2$ | 2 | 6 | $A, B$ |
| | | | | $C_i$ | 2 | 6 | $A_u$ |
| | | | | $C_s$ | 2 | 6 | $A', A''$ |
| $D_3$ | 6 | $E$ | 1 | $C_2$ | 2 | 3 | $A, B$ |
| $D_{2d}$ | 8 | $E$ | 1 | $D_2$ | 4 | 2 | $B_2, B_3$ |
| | | | | $C_{2v}$ | 4 | 2 | $B_1, B_2$ |
| | | | 2 | $C_2$ | 2 | 4 | $B$ |
| $S_{10}$ | 10 | $E_{1g}$ | 1 | $C_i$ | 2 | 5 | $A_g$ |
| | | $E_{2g}$ | 1 | $C_i$ | 2 | 5 | $A_g$ |
| | | $E_{1u}$ | 1 | $C_i$ | 2 | 5 | $A_u$ |
| | | $E_{2u}$ | 1 | $C_i$ | 2 | 5 | $A_u$ |
| $S_8$ | 8 | $E_1$ | 2 | $C_2$ | 2 | 4 | $B$ |
| | | $E_2$ | 1 | $C_4$ | 4 | 2 | $B$ |
| | | $E_3$ | 2 | $C_2$ | 2 | 4 | $B$ |
| $S_6$ | 6 | $E_g$ | 1 | $C_i$ | 2 | 3 | $A_g$ |
| | | $E_u$ | 1 | $C_i$ | 2 | 3 | $A_u$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| $S_4$ | 4 | $E$ | 1 | $C_2$ | 2 | 2 | $B$ |
| $C_8$ | 8 | $E_1$ | 2 | $C_2$ | 2 | 4 | $B$ |
| | | $E_2$ | 1 | $C_4$ | 4 | 2 | $B$ |
| | | $E_3$ | 2 | $C_2$ | 2 | 4 | $B$ |
| $C_{6h}$ | 12 | $E_{1g}$ | 1 | $C_{2h}$ | 4 | 3 | $B_g$ |
| | | | 2 | $C_2$ | 2 | 6 | $B$ |
| | | | | $C_i$ | 2 | 6 | $A_g$ |
| | | | | $C_s$ | 2 | 6 | $A''$ |
| | | $E_{2g}$ | 1 | $C_{2h}$ | 4 | 3 | $A_g$ |
| | | | 2 | $C_2$ | 2 | 6 | $A$ |
| | | | | $C_i$ | 2 | 6 | $A_g$ |
| | | | | $C_s$ | 2 | 6 | $A'$ |
| | | $E_{1u}$ | 1 | $C_{2h}$ | 4 | 3 | $B_u$ |
| | | | 2 | $C_2$ | 2 | 6 | $B$ |
| | | | | $C_i$ | 2 | 6 | $A_u$ |
| | | | | $C_s$ | 2 | 6 | $A'$ |
| | | $E_{2u}$ | 1 | $C_{2h}$ | 4 | 3 | $A_u$ |
| | | | 2 | $C_2$ | 2 | 6 | $A$ |
| | | | | $C_i$ | 2 | 6 | $A_u$ |
| | | | | $C_s$ | 2 | 6 | $A''$ |
| $C_{6v}$ | 12 | $E_1$ | 1 | $C_{2v}$ | 4 | 3 | $B_1, B_2$ |
| | | | 2 | $C_2$ | 2 | 6 | $B$ |
| | | | | $C_s$ | 2 | 6 | $A', A''$ |
| | | $E_2$ | 1 | $C_{2v}$ | 4 | 3 | $A_1, A_2$ |
| | | | 2 | $C_2$ | 2 | 6 | $A$ |
| | | | | $C_s$ | 2 | 6 | $A', A''$ |
| $C_6$ | 6 | $E_1$ | 1 | $C_2$ | 2 | 3 | $B$ |
| | | $E_2$ | 1 | $C_2$ | 2 | 3 | $A$ |
| $C_{5h}$ | 10 | $E_1'$ | 1 | $C_s$ | 2 | 5 | $A'$ |
| | | $E_2'$ | 1 | $C_s$ | 2 | 5 | $A'$ |
| | | $E_1''$ | 1 | $C_s$ | 2 | 5 | $A''$ |
| | | $E_2''$ | 1 | $C_s$ | 2 | 5 | $A''$ |
| $C_{5v}$ | 10 | $E_1$ | 1 | $C_s$ | 2 | 5 | $A', A''$ |
| | | $E_2$ | 1 | $C_s$ | 2 | 5 | $A', A''$ |
| $C_{4h}$ | 8 | $E_g$ | 1 | $C_{2h}$ | 4 | 2 | $B_g$ |
| | | | 2 | $C_2$ | 2 | 4 | $B$ |
| | | $E_u$ | 1 | $C_{2h}$ | 4 | 2 | $B_u$ |
| | | | 2 | $C_2$ | 2 | 4 | $B$ |
| $C_{4v}$ | 8 | $E$ | 1 | $C_{2v}$ | 4 | 2 | $B_1, B_2$ |
| | | | 2 | $C_2$ | 2 | 4 | $B$ |
| $C_4$ | 4 | $E$ | 1 | $C_2$ | 2 | 2 | $B$ |
| $C_{3h}$ | 6 | $E'$ | 1 | $C_s$ | 2 | 3 | $A'$ |

*Table 1* (Continued)

| Group | Order | Electron term | Level | Subgroup | Order of subgroup | Number of equivalent extremal points | Stable electron term |
|---|---|---|---|---|---|---|---|
| | | $E''$ | 1 | $C_s$ | 2 | 3 | $A''$ |
| $C_{3v}$ | 6 | $E$ | 1 | $C_s$ | 2 | 3 | $A', A''$ |

*a*) Notation for irreducible representations:

1. $A$: 1-Dimensional representation which is symmetric with respect to rotation about the principal axis;
   $B$: 1-dimensional representation which is antisymmetric with respect to rotation about the principal axis;
   $E$: 2-dimensional representation;
   $T$: 3-dimensional representation;
   $G$: 4-dimensional representation;
   $H$: 5-dimensional representation.
2. Subscript 1, 2:
   For $A$ and $B$ representations only-symmetric (1) or antisymmetric (2) with respect to $C_2$ axis perpendicular to the principal axis, or, in the absence of this, with respect to a vertical symmetry plane.
3. If there exist higher subscripts (3, 4 or 5), these indicate the different symmetry with respect to specific symmetry operation, which depends on the given symmetry group (for example in the groups $D_{6d}$, $D_{4d}$, $D_{2h}$, $S_8$).
4. Primes and double primes (′ and ″):
   Where appropriate, these indicate symmetry (′) or antisymmetry (″) with respect to a horizontal mirror plane.
5. g and u subscripts:
   Where appropriate, these denote symmetry (g — gerade) or antisymmetry (u — ungerade) with respect to an inversion centre.

If these rules allow several different labels, g and u take precedence over 1 and 2, which take precedence over  and ″

## Discussion

We start our discussion by presenting the scheme for the octahedral symmetry group ($O_h$). Its order is equal to 48 and contains 6 multi-dimensional irreducible representations ($E_g$, $E_u$, $T_{1g}$, $T_{2g}$, $T_{1u}$, and $T_{2u}$). It contains all together 24 subgroups ($O$, $T_d$, $T_h$, $D_{4h}$, $D_{3d}$, $D_4$, $D_3$, $D_2$, $D_{2h}$, $D_{2d}$, $S_6$, $S_4$, $T$, $C_{3v}$, $C_{2h}$, $C_{4v}$, $C_{4h}$, $C_{2v}$, $C_4$, $C_3$, $C_2$, $C_i$, $C_s$, and $C_1$). The following subgroups fulfil the three above-mentioned conditions: $D_{4h}$, $D_{3d}$, $D_4$, $D_3$, $D_2$, $D_{2h}$, $D_{2d}$, $S_6$, $C_3$, $C_2$, $C_{2h}$, $C_{2v}$, $C_i$, and $C_s$. In the case of three-times degenerate $T_{2g}$ electron term this is in the first level split to $B_{2g}$ and $E_g$ terms in the subgroup $D_{4h}$ or to terms $A_{1g}$ and $E_g$ in the subgroup $D_{3d}$. The

other three direct subgroups ($O$, $T_h$, and $T_d$) do not cause splitting of $T_{2g}$ electron term. In the second level the degenerate representations of the first level split to the following nondegenerate irreducible representations: $B_2(D_4)$, $A_1(D_3)$, $B_1(D_{2d})$, $B_{1g}$, $B_{2g}$, and $B_{3g}(D_{2h})$, $A_g(S_6)$, $A_1(C_{3v})$, $A_g$ and $B_g(C_{2h})$. In the third level the degenerate irreducible representations of the second level split to the following nondegenerate irreducible representations: $B_1$, $B_2$, and $B_3(D_2)$, $A(C_3)$, $B_1$ and $B_2(C_{2v})$, $B_g(C_{2h})$, $A$ and $B(C_2)$, $A_g(C_i)$, $A'$ and $A''(C_s)$. In the fourth level we have only one nondegenerate irreducible representation $B(C_2)$.

If we limit ourselves to the so-called Jahn—Teller active vibrations which give already the nonzero contribution to vibronic interaction in the first order of perturbation theory, it is sufficient to take into account only the centro-symmetric vibrations. In this case we can limit ourselves only to the subgroups which possess the inversion symmetry operation. Such are only the subgroups $D_{4h}$, $D_{3d}$, $S_6$, $D_{2h}$, $C_{2h}$, and $C_i$. Through this limitation we get in the first level the irreducible representations $B_{2g}(D_{4h})$ and $A_{1g}(D_{3d})$. In the second level we get $B_{1g}$, $B_{2g}$, and $B_{3g}(D_{2h})$, $A_g$ and $B_g(C_{2h})$, and $A_g(S_6)$ irreducible representations. In the third level we have only $B_g(C_{2h})$ and $A_g(C_i)$ irreducible representations. For octahedral system in three-times degenerate $T_{2g}$ electron term using this limitation we get:

| | |
|---|---|
| i) three equivalent geometries of $D_{4h}$ symmetry<br>ii) four equivalent geometris of $D_{3d}$ symmetry | 1st level |
| iii) six equivalent geometries of $D_{2h}$ symmetry<br>iv) eight equivalent geometries of $S_6$ symmetry<br>v) twelve equivalent geometries of $C_{2h}$ symmetry | 2nd level |
| vi) twelve equivalent geometries of $C_{2h}$ symmetry<br>vii) twenty-four equivalent geometries of $C_i$ symmetry | 3rd level |

It is necessary to note that conclusions based on assuming only the centro-symmetric subgroups are valid only in the first order of perturbation theory. Therefore in some approaches [1—19] this limitation occurs.

The classification of molecular symmetry point groups according to given rules (presented in Table 1) determines all the possible symmetries of systems which undergo the Jahn—Teller deformation. The presented table therefore represents the complete classification of possible symmetries of Jahn—Teller systems for all symmetry point groups of molecules. Thus the existence of deformations of formerly symmetric system into the system of different symmetry cannot be due to the Jahn—Teller effect. On the basis of group theory we can reject also some commonly used explanations of the transition between some geometries as the consequence of Jahn—Teller effect. Therefore for example the transition tetrahedron (symmetry $T_d$)↔square planar (symmetry $D_{4h}$) cannot be due to the Jahn—Teller effect, because the group $D_{4h}$ (order 16) is not subgroup of $T_d$ group (order 24). Besides, in some recent papers [19] this transition is explained as due to the Jahn—Teller effect. Similarly the transition of five-coordinated complexes

between trigonal bipyramid (symmetry $D_{3h}$) and square pyramid (symmetry $C_{4v}$) is not due to Jahn—Teller deformation because group $C_{4v}$ (order 8) is not subgroup of $D_{3h}$ group (order 12).

On the other hand, we must have in mind also the limitation of group-theoretical approach to the solution of problems of symmetries of Jahn—Teller systems. Such an approach on one side gives the geometries of all possible extremal points of adiabatic potential for given system but on the other side it says nothing whether these extremal points will be realized or not.

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