CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2023, 18(2), 7-14
ISSN (p) 1857-1727 ISSN (e) 2345-1688
http://cjm.ichem.md
http://doi.org/10.19261/cjm.2023.1098

SPONTANEOUS SYMMETRY BREAKING AS A LAW OF NATURE

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Abstract. In a semi-review paper, it was discussed the notion of symmetry of polyatomic systems defined as invariance under transformations, and show that this important property of atomic matter is extremely vulnerable, and may undergo internal breakdown, subject to the presence of electronic degeneracy or pseudodegeneracy. First formulated by Landau, L. in 1934, later proved and published by Jahn and Teller, this Jahn-Teller effect (JTE) underwent tremendous developments with important applications in physics, chemistry, biology, and materials science. Less attention was paid to the roots of this phenomenon and its correct interpretation in the sense of its influence on observable properties. It is shown that electronic degeneracy and its extended form, called pseudodegeneracy, are actually the only source of spontaneous symmetry breaking (SSB) in nature, including all forms of matter, beginning with elementary particles, via nuclei, atoms, molecules, and solids. Theoretically, the vulnerability of the notion of symmetry is due to the fact that, following quantum mechanics, the separation of the motion of electrons and nuclei (and, similarly, the separation of motions of elementary particles) is approximate, and hence the classical notion of polyatomic space configuration is approximate too, with SSB as one of its main violation.

Keywords: adiabatic potential, electronic degeneracy, Jahn-Teller effect, pseudo Jahn-Teller effect, spontaneous symmetry breaking.

Received: 25 August 2023

Background

Symmetry is one of the most widespread characteristics of systems and processes in the material world and humane relations, and it plays an outstanding role in science, engineering, aesthetics, arts, and everyday life [1-3]. In science, the motion of the units of atomic matter (atoms, molecules, solids, elementary particles) are described by equations that obey some well-known symmetries, meaning they remain invariant with respect to a variety of transformations (*e.g.*, rotations, reflections, translations, permutations, time reversal, and Lorenz and gauge transformations) [1,2]. In general, symmetry is invariance under transformation. Actually, all the statements of symmetry invariances in atomic matter are grounded in the global assumption that space is isotropic and homogeneous, and time is uniform.

The role of symmetry invariance in science is exceptional. Not only are we able to rationalize the origin of observable properties based on symmetry principles, but we can also predict new laws and new observable properties based on the requirement of symmetry invariance. Following Einstein, A. "*It is now natural for us to derive the laws of nature and to test their validity by means of the laws of invariance, rather than to derive the laws of invariance from what we believe to be the laws of nature.*" [4].

At first sight, symmetry invariances are due to the general laws of isotropic space and uniform time, but in real Universe the majority of macro and micro objects and the Universe itself (the "Vacuum" [5,6]) do not obey the highest possible symmetry: they are in a state of broken symmetry. Broken symmetry of any object (system) is easily induced by external perturbations, but there are many cases when the symmetry is broken by internal forces, it takes place spontaneously, without external influence. Spontaneous symmetry breaking (SSB) in atomic matter implies that a high-symmetry configuration of the systems is plausible (may be expected), but it shows a configuration with lower symmetry in equilibrium, the symmetry breaking taking place under internal forces only.

SSB in matter are very important, as they are present (explicitly or implicitly) in the majority of processes, including a variety of physical, chemical, and biological phenomena based on molecular configuration instability, and all kinds of phase transitions [7-10], as well as in the very existence of some elementary massive particles [5,6]. With regard to the properties of atomic matter, SSB plays a fundamental role: in the majority of polyatomic systems, equilibrium configuration acquires a variety of symmetries with observable geometries away from the possible high-symmetry configurations [11].

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What is the origin of SSB in polyatomic systems? Are there general laws controlling all SSB in atomic matter? SSB take place also in elementary particle transformations, as well as in transitions from elementary particles to nuclei, to atoms, to molecules and solids, and under phase transitions in solids (see below). Are all these SSB independent or interdependent by some general property related to matter? With regard to atomic matter, in simple cases (*e.g.,* triatomic molecules) the SSB can be attributed to quantized low-symmetry electronic distributions and hybridizations, but this simplified picture does not work in more complicated situations. It comes out that there is a more general law of Nature that controls all the SSB: degeneracy and pseudodegeneracy [7-13] (local quantized orbitals and hybridizations demonstrate the local forces which combine to produce the degeneracies that drive the SSB). In other words, it looks like "*Nature tries to avoid polyatomic equilibrium space-configurations that produce two or more close-in-energy states*" (a part of this idea and some of its consequences were discussed in earlier publications [11-13]).

Degeneracies and SSB in polyatomic systems: the Jahn-Teller effects. Quantum definition of stereo-chemical space configuration

The fundamental property of polyatomic system to undergo spontaneous symmetry breaking induced by degeneracy, presently known as the Jahn-Teller effect (JTE), was first formulated by Landau, L. in 1934 as follows: the configuration of any nonlinear polyatomic system in a degenerate electronic state undergoes spontaneous distortions that remove the degeneracy [14]. Since then, many extensions of this groundbreaking idea were revealed and developed. Figure 1 illustrates the studied so-far four modifications of the Jahn-Teller effects (JTEs), which include the original JTE, pseudo-JTE, hidden-JTE, and hidden-PJTE, by visualization of the cross-sections of their adiabatic potential energy surfaces (APES) in the simplest cases when there is only one coordinate of distortion [15]. When there is more than one coordinate of instability and distortion, these APES acquire more complicated forms with several (or an infinite number of) equivalent minima [7-10].

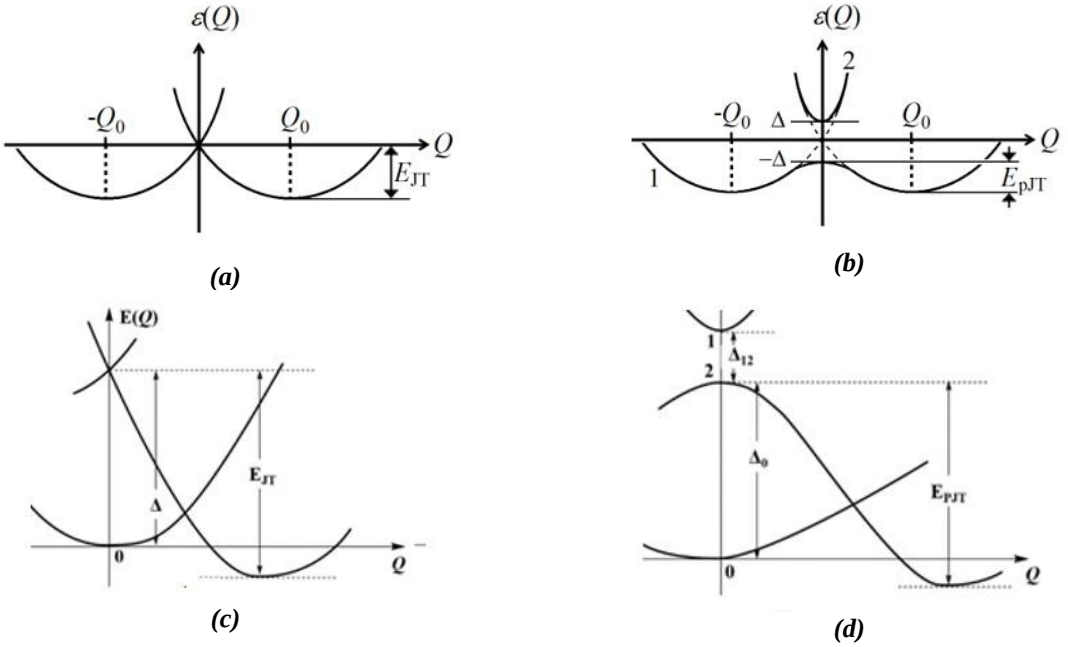


Figure 1. Illustration to the definition of the four types of electronic configurations causing the four kinds of Jahn-Teller effects; for simplicity, in all four cases only one symmetrized coordinate *Q* of the low-symmetry nuclear displacements from the reference high-symmetry configuration at *Q*=0 is shown; E_{JT} and E_{PJT} are the JTE stabilization energies, and Δ denotes energy gaps. In the case of proper JTE the system is unstable, it has no minimum of the adiabatic potential energy surface (APES) at the point of electronic degeneracy *Q*= 0, but it may be stable in the distorted configurations at ±Q_0 *(a).* The pseudo-JTE (PJTE) case: there is no degeneracy at *Q*= 0, but the system is unstable (the curvature *K* of the ground-state APES is negative) due to the pseudodegeneracy caused by strong vibronic coupling *F* to low-lying excited states at Δ< F^2/K_0 (see the text) *(b).* Hidden-JTE: there is neither degeneracy nor pseudodegeneracy in the ground state of the system, but there is a sufficiently low-lying excited state that has a JTE, which is so strong, E_{JT}> Δ, that it penetrates the high-symmetry ground state, producing a global minimum with a distorted configuration *(c)*. Hidden-PJTE: the same situation as in the hidden-JTE, but the intervening excited state has a strong PJTE, instead of the JTE *(d)*.

With all these modifications of the JTEs included, we conclude that there are no polyatomic systems that can a priori be excluded from the possibility of spontaneous symmetry breaking (SSB). Moreover, it was proved that the JTE and the PJTE are the only source of instability and spontaneous distortions of high-symmetry configurations of polyatomic systems [7,8,16,17]. Actually, as discussed below, degeneracy and pseudodegeneracy are the only source of SSB in the whole spectrum of transformations in matter, from elementary particles to nuclei, to atoms, molecules and solids [11,12,18].

As illustrated above in Figure 1, in all the four modifications of the JTEs, starting with a high-symmetry configuration in a given electronic state, the instability and consequent SSB take place due to the present of other active electronic states involved in the process. In other words, in all the cases of JTEs, there are two or more electronic states, which are coupled by the nuclear displacement, leading to SSB; it illustrates the idea that SSB in all these cases are directly related to degeneracy or pseudodegeneracy. They emerge from the first principles of quantum mechanics as due to the non-adiabatic contribution to the interactions between the electrons and nuclei [7,8].

Strictly speaking, the emergence of SSB in polyatomic systems, which leads to the multiminimum nature of the APES, requires a revision of the "classical" notion of polyatomic space configuration (molecular shapes, crystal local and bulk structures, clusters, two-dimensional systems, thin films, quantum dots, qubits, *etc.*) and related properties. Indeed, in quantum-mechanical description of the motions of the electrons and nuclei, the notion of space configuration is introduced in the adiabatic approximation, in which it is assumed that due to the huge difference between the masses of electrons and nuclei, the fast moving electrons follow adiabatically the much slower nuclear motions (here adiabatic means that at each instantly fixed nuclear configuration, a stationary electronic charge distribution is achieved, while the nuclei move in the averaged field of the electrons). Under these conditions, the description of the motions of nuclei and electrons can be (approximately) separated. Then, by calculating the energy of the system as a function of nuclear coordinates, the APES, one finds the points of minimum energy. The nuclear coordinates at these points define the local equilibrium configuration of the system.

But the adiabatic approximation is (very often) violated, thus questioning the accuracy of the classical definition of polyatomic configurations as stable geometrical formations at equilibrium. The adiabatic approximation is especially vulnerable and may be significantly violated when for a given nuclear configuration there are the mentioned above two or more close in energy, degenerate or relatively near-degenerate (pseudodegenerate), electronic states that become mixed (coupled) under nuclear displacements. Indeed, in these cases, in classical language, "the electrons have additional "degrees of freedom" that allows them to avoid (partially) the necessity to follow adiabatically the slower nuclear displacements (in first-principle calculations, the off-diagonal matrix elements of the operator of nonadiabacity that involves two or more electronic states acquires significant values [7]), thus violating the adiabatic approximation and the accuracy of the notion of nuclear configuration: there is no minimum of the APES at these points. The JTE and PJTE emerge as the corrections to the notion of polyatomic configuration, which compensate for the violation of the adiabatic approximation.

The JTEs provide for a general (rigorous) explanation of the origin of all SSB in polyatomic systems, for which the notion of space configuration is valid. With these effects included we get the improved (quantum) definition of polyatomic space configuration. Under this definition "there are three types of polyatomic configurations with significant differences in related observable properties with regard to SSB. To the first type belong polyatomic systems in stable high-symmetry configurations with no electronic degeneracy or pseudodegeneracy in the ground and low-lying excited states, and hence no explicit or hidden JTE and PJTE, meaning systems with negligible structural non-adiabacity. For these systems, the improved definition coincides with the widespread "classical" meaning of configurations that are stable in the classical high-symmetry nuclear arrangement, but with significant limitations of systems, to which this definition applies, making them rather exceptional.

The second type of systems are those with instabilities of the high-symmetry configuration induced by the JTE and PJTE, as well as the hidden JTE and PJTE, resulting in SSB with small to moderate distortions, the latter being of dynamic nature. Because of these effects, assumed static configurations (with small normal vibrations) become configurational-dynamic, due to two or several, or an infinite number of equivalent minima of the APES. These are the systems with a rich variety of novel

properties, partially demonstrated in books and reviews [7-11].

The third group of systems are those with very strong non-adiabacity in the high-symmetry configuration, for which the JTEs result in two or several equivalent, or in an unlimited number of equivalent distorted configurations (in a trough), with a very high stabilization energy by distortion. The systems under this definition, once created in the distorted configuration, remain there forever, and in this respect, they do not challenge the classical image of a stable low-symmetry configuration. For these cases, the larger definition tells one why the system is not in its possible high-symmetry configuration, and more specifically, what is the origin of its deviation from the (plausible) high-symmetry configuration in terms of JTEs parameters.

Polyatomic systems of the second group with relatively easily observable SSB dynamics in the space configuration possess a gamma of special properties, known as JTEs. Compounds of the first group with stable high-symmetry configurations and the third group with stable low-symmetry configurations, at first sight, fully coincide with their widespread "classical" definitions. However, the knowledge that their stabilities are just particular cases of polyatomic configuration with either very weak nonadiabacity (as in the compounds of the first group), or very strong nonadiabacity (in the third group), is very important, as it allows for manipulations of their properties by means of external influence. Indeed, as mentioned above, the nonadiabacity is directly reflected in the JTEs parameters (degeneracies and pseudodegeneracies, energy gaps, vibronic coupling constants, primary force constants [7,8]). Direct manipulation of structural properties of systems from the third group was realized by means of external influence targeting their JTEs parameters [5-6,11-13].

Note, that there are no distinct borders between the three groups of compounds, and it is not always known a priori to which group the system under consideration belongs. For example, "the ammonia molecule NH_3 is unstable in the high-symmetry planar configuration because of the PJTE instability of the latter, but the moderate barrier between the two equivalent pyramidal structures allows for the tunneling between them, a non-classical property, making this system pertain to the second group. However, in a very similar molecule AsH_3 with formally the same, but much stronger PJTE in the planar geometry, the barrier between the distorted pyramidal configurations becomes too large with the tunneling frequency negligible, so its configuration belongs to the third group of well-defined classical low-symmetry structures. In between these two examples, there is a similar molecule, PH_3, with very slow (but still observable) tunneling effect, reflecting the blur border between the three groups of configurations, defined above [9].

Degeneracy and SSB in all transformations of atomic matter: Nature strives to avoid degeneracies by means of symmetry breaking

The understanding on how degeneracy leads to SSB in polyatomic systems and, vice versa, that all the SSB in polyatomic systems are due to, and only to degeneracies, was extended to include all the spontaneous transformations in atomic matter [11,12], meaning formation of molecules from atoms in the gas phase, and gas phase-liquid, liquid-solid, and between solid state phase transitions. Together with the well-known statement in particle physics that "*elementary particle transformations are always associated with a degeneracy*" [5,6], it came be generalized in to the conclusion that "*Nature strives to avoid degeneracies by means of symmetry breaking*" [11-13].

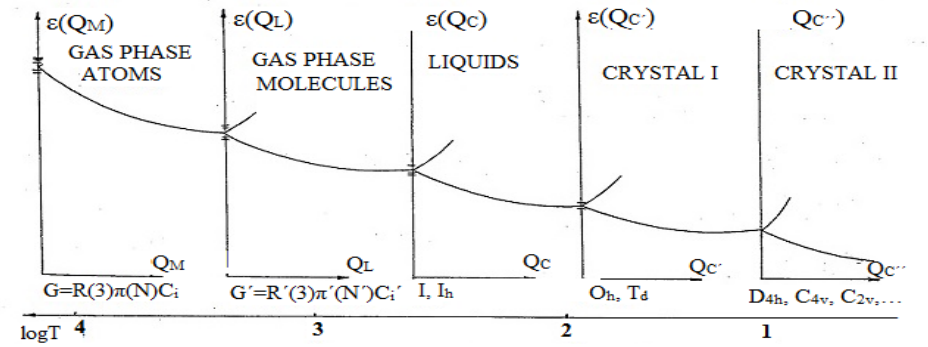


Figure 2. Illustrative scheme for the cascade of degeneracy-- and pseudodegeneracy--induced transformations from atoms to molecules to liquids to solids and within solids as a function of temperature logT, illustrating the idea of consequent SSB when the appropriate degree of degeneracy is reached by cooling. The normal coordinates of distortion Q_Γ and the decreasing rotational R(3), permutation π(N), inversion C_i, icosahedral, cubic, and tetragonal symmetries are shown on the abscise axes [11].

Figure 2 illustrates schematically how degeneracy leads to SSB in phase transitions in atomic matter (for thermodynamic details of the process see [11]). Starting with matter in the form of atoms, which at high temperatures are separated (no degeneracy because of the high-frequency vibrational dissociative states), by cooling reaches an interaction configuration with appropriate degeneracy (pseudodegeneracy) that leads to SSB with formation of molecules. Similarly, by further cooling, the gas molecules acquire interactional states with degeneracies that lead consecutively to lower symmetry liquid state, crystallization, and crystal phase transitions [11,12].

Some general consequences from the SSB law of Nature

To reformulate the SSB law of Nature under consideration, we state that, in spite of the Nature's isotropic and homogenous space and uniform time, the symmetry of the units of atomic matter (elementary particles, nuclei, atoms, and polyatomic systems) is not preserved, it undergoes spontaneous breaking, subject to degeneracy and pseudodegeneracy. On the other hand, if there is any observable SSB in atomic matter, it is due to, and only to degeneracies. This SSB law has important far-going consequences for natural sciences with applications in physics, chemistry, biology, materials science and engineering [7-10].

For many years this SSB law was considered mostly by its main consequences in studying space configurations of polyatomic systems and their distortions, known as the Jahn-Teller effects (JTEs). The applications and the novel findings based on these effects are innumerable. They grew up from particular features to general tools in exploring the structure and properties of molecular systems and solids [9,10]. Among the latest achievements in this respect, we mention here the application of the specific features of the JTEs to the study of impurity centers in diamond in application as qubits in quantum computation and information storage [19], use of information about the electronic structure of the local canters in crystals to induce or quench their local JTEs and related observable properties by means of external influence (the idea was realized on a hexaferrite crystal, inducing the JTE in its whole sublatice of tetrahedral non-JT centers by inserting a limited concentration of electron-donor Ti impurities [20]). Similarly, additional donor atoms were used in planarization of two-dimensional system *via* influencing the PJTE on its centers, which originates the puckering (buckling) of the system [21,22]. A series of important applications emerged from the studies of the cooperative JTEs in crystals, including the origin of spontaneous polarization and order-disorder phase transitions, ferroelectricity, multiferroicity, flexoelectricity, permittivity and orientational polarization [23-25].

A novel (global) trend in this field started developing recently, although its possibilities were indicated earlier [26-30]. The point is about all the atomic-matter transformations in Nature that take place involving an energy barrier, an intermediate (activation) state. It includes almost all chemical reactions, biological transformations, and a variety of physical processes (perhaps, this trend may include also other global processes in Nature that follow a similar profile). The background idea of this trend is illustrated in Figure 3*(a)*. Figure 3*(a)* shows an ubiquitous picture of how the mentioned transformations of atomic matter from stable "reactants" to stable "products" take place *via* an energy barrier. In the right-hand part the same energy curve is upended with its most important basic (unalienable) features that follow from the outlined above general SSB law of nature, according to which in this case the instability at the maximum of the transition barrier is due to a pseudodegeneracy, leading to the PJTE.

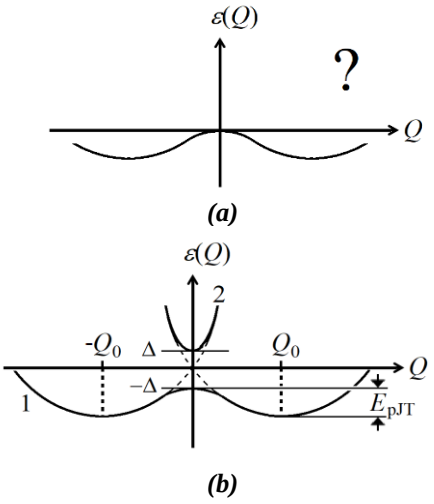


Figure 3. Typical (schematic, overwhelmingly used) picture for the changes in the potential energy (PE) of a polyatomic system that undergoes a transformation from stable "reactants" (left minimum of the PE) to stable "products" (right minimum) in overcoming a potential barrier between them (the activation energy) as a function of the generalized coordinate of transformation *Q (a).*
Correct presentation of the process taking into account the SSB law that attributes the instability at the maximum of the barrier to a pseudodegeneracy yielding the PJTE: compared with the 3*(a)* Scheme, it provides for the background origin and correct understanding of the nature of the transformation that influences all its observable characteristics *(b)*.

Obviously, all the novel parameters of this transformation, revealed by taking into account the PJTE origin of its transition state instability (some of which are shown in Figure 3*(b)*), directly influence the observable properties of the system related to the process. The main innovation factor in this treatment is the presence of a stable excited state of the intermediate (activation) complex, which characterizes its structure and properties via several relations of the PJTE [8]. First, the very present of the vibronic coupled excited state, and hence the picture as a whole, are strongly dependent on the energy gap 2Δ to the latter at the maximum of the barrier, defining the condition of the ground state instability,

$$\Delta < F^2/K_0 \qquad (1)$$

where the matrix element $F = \langle 1|(\partial H/\partial Q)_0|2\rangle$, the vibronic coupling constant, is an important characteristic of the PJTE, which depend of the nature of the interacting states and their electronic properties, and K_0 is the primary force constant (the stiffness before the vibronic coupling) in the transition state with respect to the Q displacements. For the minima positions were get [8]:

$$\pm Q_0 = [(F^2/K_0^2) - (\Delta^2/F^2)]^{1/2} \qquad (2)$$

with the minima depths – PJTE stabilization energy – which is also the transformation barrier height,

$$E_{PJT} = (F^2/2K_0) + (\Delta^2 K_0/2F^2) - \Delta \qquad (3)$$

and the curvature at the minima points defining the vibrational frequencies,

$$K = K_0[1 - (\Delta K_0/F^2)^2] \qquad (4)$$

Wide application of this novel approach to chemical (and related) transformations is just beginning [26-30]. As an example, we mention here the application of this approach to the problem of "sudden polarization" in photochemistry, where the reactivity of organic molecules increases significantly by photoexcitation [30]. By employing the above PJTE theory, it was shown that the activation of the excited state is due to the PJTE involving the next higher close-in-energy) electronic states, as shown in Figure 4. Application to the stilbene molecule is illustrated in Figure 5.

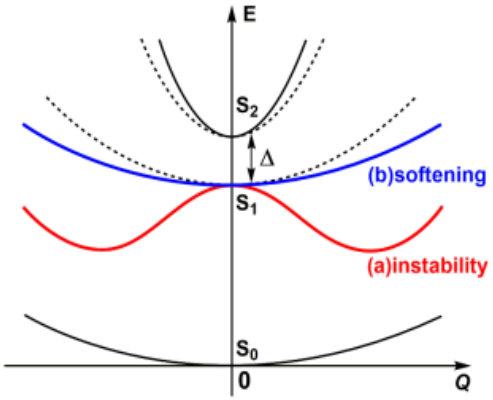


Figure 4. The PJTE in the excited state S1 explains the origin of "sudden polarization" as due to the presence of a next, close-in-energy excited state that leads to either softening (blue curve) or instability (red curve), provided the condition (1) is obeyed.

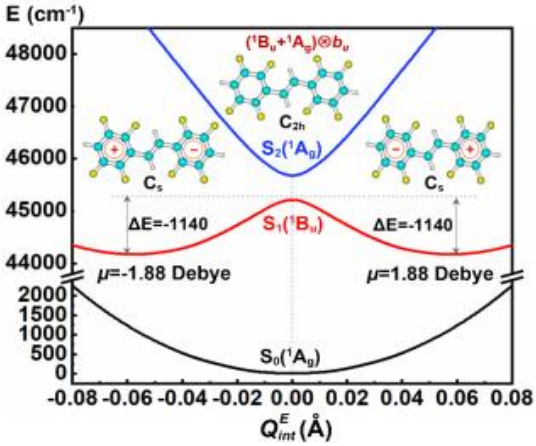


Figure 5. *Ab initio* calculations performed on the stilbene molecule confirm the origin of its photochemical "sudden polarization" resulting in the zwitterion structure, as due to the PJTE in the excited state [30].

Conclusions

The statement that electronic degeneracy (including pseudodegeneracy) is the only source of spontaneous symmetry breaking (SSB) in atomic matter, formulated as a law of Nature, is very strong, with many consequences for the structure and properties of polyatomic systems. The best known of them are the Jahn-Teller effects in their four modifications with many applications in exploring physical, chemical, and biological phenomena, and in materials science. Among the latest innovation in this field we emphasize here the importance of *the origin of transition states of chemical reactions and related processes as due to the PJTE*.

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Short biography of the author



Academician Isaac Bersuker is the founder of the Quantum Chemistry Laboratory within the Institute of Chemistry of the Academy of Sciences of Moldova, at the head of which he was for almost a quarter of a century (1969-1993); founded the Scientific School of Quantum Chemistry in the Republic of Moldova at the end of the 1980s and is one of the world's best-known researchers of the theory of the Jahn–Teller Effect (JTE) and the Pseudo Jahn–Teller Effect (PJTE). He predicted tunnel splitting in JT systems, demonstrated that JT and PJT effects are the only source of spontaneous symmetry breaking (SSB) in polyatomic systems, identified hidden JT and PJT effects, predicted the coexistence of trigonal and tetragonal distortions in the JTE for the T term, created the vibronic theory of ferroelectricity in cubic perovskite, discovered the role of spin in the spontaneous polarization of crystals and new classes of multiferroics with magnetic-ferroelectric crossover, revealed the role of JT and PJT effects in mixed-valence compounds, developed methods of evaluation of JT effect parameters from ultrasound experiments. In 1993, he became a senior research scientist and professor at the Department of Chemistry of the University of Texas at Austin, USA, being the doctoral and post-doctoral supervisor of 31 students and doctors.

Academician Isaac Bersuker is the doctoral and post-doctoral supervisor of 31 students and doctors. He is the author of 15 monographs and more than 600 scientific works. His books on JTE and PJTE, published in 1984, 1989, 2006 and 2010 are the most influential in world science.

Academician Isaak Bersuker is the first laureate of the State Prize of the Republic of Moldova in the field of science and technology (1980), he is decorated with the "Order of Honor" (2004), the Medal "L.A. Ciugaev" of the Russian Academy of Sciences, the "David Ben-Gurion" Medal (2005, Israel), the "Scientific Merit " Medal (2021), the Academy of Sciences of Moldova Medal "Nicolae Milescu Spătarul" (2023).

Theoretical physicist, research field: quantum chemistry, physics and chemistry of solid state, theory of Jahn-Teller, pseudo Jahn-Teller and Renner-Teller effects, vibronic interactions and a wide variety of their applications.

Doctor habilitate in physical and mathematical sciences (1964), member of the Academy of Sciences of Moldova (1989), professor at the Department of Chemistry, University of Texas at Austin (since 1993).