Hermann Jahn and Rudolf Renner of the Jahn–Teller and Renner–Teller effects

Magdolna Hargittai · István Hargittai

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Abstract Vibronic interactions have received increasing attention in modern structural chemistry. Edward Teller played a pioneering role in understanding and describing them during the “molecular physics” period of his scientific career. Very little is known about the two scientists who contributed significantly to our knowledge about these effects and whose names have become associated with Teller’s. This Editorial is devoted to Hermann Jahn and Rudolf Renner and attempts to lift them out of oblivion by paying them tribute for their contributions.

Keywords Hermann Jahn · Jahn–Teller effect · Rudolf Renner · Renner–Teller effect · Edward Teller · Vibronic interactions · Born–Oppenheimer approximation

During the 62 years since its publication [1] the importance of the Jahn–Teller effect has grown substantially; partly due to its importance in high- T_c superconductivity [2]. According to the original formulation of the Jahn–Teller effect, a non-linear symmetrical molecule with a partially filled set of degenerate orbitals is unstable and gets distorted, thereby removing the electronic degeneracy until a non-degenerate ground state is achieved. In simpler terms, in such a molecule there is a mismatch between the high

Left: Hermann A. Jahn (1907–1979; in the early 1930s; courtesy of Michael Jahn and Margaret May, Jahn’s son and daughter, London) and *right:* Rudolf Renner (1909–1991; courtesy of Beate Bauer-Renner, Rudolf Renner’s daughter-in-law, Dorum, Germany)

symmetry of the ensemble of the atomic nuclei and the lower symmetry of the electron density distribution and this causes some of the nuclei to move from their original positions into ones that match the symmetry of the electron density distribution and, as a consequence, the symmetry of the molecule decreases. Since the Jahn–Teller effect entails the coupling of the electronic and vibrational motions of a molecule, it represents a breakdown of the well-known Born–Oppenheimer approximation, according to which the electronic and vibrational motions of a molecule can be separated because the relatively heavy nuclei move much more slowly than do the electrons. Thus, it can be assumed that the latter move about a fixed nuclear arrangement [3].

That the Jahn–Teller effect does not apply to linear molecules is simply due to an inconsistency between the symmetry of the degenerate electronic state and the symmetry of the vibration that can take the molecule out of the

M. Hargittai · I. Hargittai (✉)
Department of Inorganic and Analytical Chemistry and Materials
Structure and Modeling Research Group of the Hungarian
Academy of Sciences, Budapest University of Technology and
Economics, P.O. Box 91, 1521 Budapest, Hungary
e-mail: istvan.hargittai@gmail.com

M. Hargittai
e-mail: hargittaim@mail.bme.hu

linear configuration, e.g., the doubly degenerate bending vibration of a linear triatomic molecule, AB_2 . There is though still a possibility for such molecules to become unstable in their linear shape and that is described by the Renner–Teller effect (*vide infra*). The Jahn–Teller and Renner–Teller effects belong to the so-called “vibronic interactions.” Although the Jahn–Teller effect is the best known among them, historically it was preceded by the discovery of the Renner–Teller effect and both of them were preceded by some related work of Edward Teller and Gerhard Herzberg.

Teller met with Herzberg, the future Nobel laureate spectroscopist, in the early 1930s in Darmstadt, Germany. More than 50 years later, Herzberg remembered vividly his interactions with Teller:

Our discussions at that meeting later led to our collaboration in the paper on the vibrational structure of electronic transitions in polyatomic molecules, which was written during visits of mine to Göttingen and visits by Teller to Darmstadt. My function was that of a midwife: Teller had the ideas, which I tried to get out of him by describing the experimental results to him and by drafting a tentative form of the paper, which he then corrected. Teller had an extraordinary reservoir of ideas in this field (as well as in other fields) and was always ready to share his knowledge. Working with him was an experience that I shall never forget. Although the ideas came from him, he insisted that on the title page we follow the alphabetical order of the authors [4].

Their still often cited paper, written on the above topic, was published in 1933 [5] and it discussed the coupling of the electronic and vibrational motions of molecules during electronic transitions. This is generally referred to as the Herzberg–Teller effect. It can certainly be considered as a forerunner of the Jahn–Teller effect. Chronologically, the paper by Renner follows (published in 1934) [6], with the description of the vibronic interaction in the first electronic excited state of CO_2 . Although, due to the above-mentioned symmetry mismatch, there is no linear coupling in this molecule, there still can be considerable quadratic coupling that can cause the molecule to bend and thus the electronic degeneracy is removed. Interestingly, it took a quarter of a century to find the first experimental evidence of the Renner–Teller effect, in the electronic absorption spectrum of the NH_2 radical [7]. The NH_2 radical has one electron on a π orbital and thus a Π electronic state in its ground state, where it is bent; while it is linear in the excited nondegenerate state.

Edward Teller and Lev Landau used to have discussions on the possibility and result of interactions between the electronic and vibrational wave functions of molecules and,

according to Teller, they argued about this question. The way he explained Landau’s contribution to this effect is interesting but also somewhat confusing. We are quoting here the relevant part of his description [8, 9]:

This effect had something to do with Lev Landau. I had a German student in Göttingen, R. Renner, and he wrote a paper on degenerate electronic states in the linear carbon dioxide molecule, assuming that the excited, degenerate state of carbon dioxide is linear.

In the year 1934 both Landau and I were in Niels Bohr’s Institute in Copenhagen and we had many discussions. He disagreed with Renner’s paper, he disliked it. He said that if the molecule is in a degenerate electronic state then its symmetry will be destroyed and the molecule will no longer be linear. Landau was wrong. I managed to convince him and he agreed with me. This was probably the only case when I won an argument with Landau.

What is confusing in this story is that Teller assumes that the degenerate excited state of CO_2 is linear—but, in fact, Renner’s paper suggested it to be bent. What makes the difference is whether the quadratic (or higher order) terms of the interaction matrix are taken into account or not. If higher order terms could be ignored, then the above quotation from Teller would be valid and, indeed, the CO_2 molecule should be rigorously linear even in its degenerate electronic state. Let us quote from the beginning of Renner’s paper here, in which he refers to earlier results about the coupling of the electronic and rotational motions in a diatomic molecule. Renner explains why the rotations and not the vibrations are coupled with the electronic motion there: “The reason for this is the high (cylindrical) symmetry with respect to the line connecting the two nuclei. This symmetry is, of course, conserved for the vibration and so inhibits a coupling between the vibrational and electronic frequencies [10].”¹ The same is true for a symmetric linear triatomic molecule like CO_2 , for which the Σ term is nondegenerate but the Π and Δ terms are degenerate. No splitting is expected for the Σ state—in case of CO_2 this is the ground state and, indeed, the CO_2 molecule is linear in its ground electronic state. For the Π term the splitting will depend quadratically on the coordinate of the bending vibration, while for the Δ term the splitting will be proportional to the fourth power of the displacement coordinate—a very small quantity—and can mostly be ignored [10].

There might be different explanations of the quote from Teller from his late years [8, 9]. Perhaps in his earlier

¹ The quotation is from the English translation of Renner’s paper [6]: “On the theory of interaction between electronic and nuclear motion for three-atomic, bar-shaped molecules”.

discussions with Landau, Teller did not take into account the possibility that the quadratic terms might also cause distortion and Landau might have thought of this possibility but did not elaborate on it [11]. It is also possible that Landau made a mistake as the story implies—but, again, as Teller himself told us, “it bothered me that he was usually not wrong, so maybe he was always right with the exception of linear molecules [8, 9].” And that made Teller ask Jahn to do the computations for all different symmetries and that eventually led to their famous paper and the emergence of the Jahn–Teller effect [1]. Of course, a trivial explanation for Teller’s late remark might be simply that he did not remember correctly the events having taken place over 60 years prior to our conversation in 1996 quoted above [8, 9].

Rudolf Renner

Rudolf Renner was born in 1909, in Schweidnitz in Silesia (then Germany, now Swidnica in Poland). He studied first in Hannover, then, from 1929, in Göttingen, where he was awarded his doctor degree in 1934. His former supervisor, Max Born, and his consultant, Teller, by then had left Germany as a consequence of the anti-Jewish legislation following the Nazi accession to power in Germany in 1933. This might have been the reason why Renner published his paper under his name alone, but it might also have been that Born and Teller would have urged him to publish alone in any case.

In preparation for his doctoral examinations, Renner had to submit an autobiography, which was dated November 1, 1933, and has been preserved in the Archives of Göttingen University. The roughly one-page handwritten document profusely thanks Born not only for scientific guidance but also for financial assistance without which Renner could not have completed his studies. For his substantial assistance in molecular vibrational spectroscopy Renner acknowledges Teller who was staying a little longer in Göttingen after Born had left. Renner notes that Professor Eucken made it possible for him to have his doctoral exams, which is a hint that his original supervisor was no longer available [12].

Teller did not know anything about Renner for a long time, until 1980, when he received a letter from his former pupil.² As the physics program in Göttingen disintegrated, Renner entered a two-year teacher’s training program, and received a teaching certificate, but could not find employment. At this time the German Reich Weather Service was looking for natural scientists and Renner entered this

service in 1936 and worked there until the end of the war. He married a pharmacist’s daughter from Dorum, Lower Saxony, in 1942. His wife’s two brothers were killed in the war and there was no one who could be the successor of his father-in-law in the pharmacy. Hence Renner acquired training as a pharmacist and took over the family business in 1950. In 1955, his wife died of cancer and later he married a pharmacist from Dorum. Renner worked in the pharmacy for 30 years and retired in 1980.

Teller expressed his sorrow in his response that Renner could not continue in physics and noted that Renner’s work was the forerunner of the Jahn–Teller effect (“Ihre Dissertation war der Vorläufer des sogenannten ‘Jahn–Teller Effekts’ von dem immer noch viel gesprochen wird”).³ He called his life “quite active,” which was certainly an understatement. He mentioned that apart from physics he also worked for Peace. It is very unlikely that Renner and Teller had any further interaction. Renner asked Teller to visit him in Dorum, but in his response Teller noted that Dorum was situated quite outside of the main thoroughfares. Apart from this single exchange of letters with Teller, Renner lived his life without ever telling his family about his “first career.” Renner died in 1991.⁴

Hermann A. Jahn

Teller and Jahn worked together at University College London on the famous paper that eventually brought vibronic interactions into the limelight. London was Teller’s last stop before he left Europe and moved permanently to the United States. In contrast to Teller, the other eponym of the Jahn–Teller effect is hardly known. The best source of information about him is the obituary by one of his former colleagues, P. T. Landsberg [13]. Jahn was of German descent. His father left Germany and settled in England in the 1890s. Jahn was born in Colchester in 1907, grew up in Lincoln and received his BSc degree in chemistry at University College London in 1928. He became interested in quantum mechanics and continued his studies in Leipzig under the supervision of Werner Heisenberg and the Dutch mathematician Bartel L. van der Waerden. He completed his doctorate in 1935 and returned to England. He worked at the Royal Institution and during the war at the Royal Aircraft Establishment. In 1943 he married Karoline Schüler, a teacher who was a Jewish refugee from Frankfurt am Main. For 2 years from 1946 he worked at the

² Letter of November 11, 1980, from Rudolf Renner to Edward Teller; Hoover Institution Archives, Stanford University.

³ Letter (undated, presumably in November 1980) from Edward Teller to Rudolf Renner; Hoover Institution Archives, Stanford University.

⁴ Letter of April 30 (2009) from Beate Bauer-Renner, Renner’s daughter-in-law.

physics department of Birmingham University under Rudolf Peierls's guidance. He was appointed Professor of Applied Mathematics at the University of Southampton in 1949 and stayed there until he retired in 1972. He died in 1979.

Jahn and Teller interacted when Teller was at University College London and Jahn at the Royal Institution. The paper they did jointly was followed by a paper by Jahn alone. Jahn published a number of other studies, mostly on the structure of molecules, especially treating molecular vibrations. He utilized his acumen in mathematics for solving problems in the theory of X-ray scattering and applied group theory to nuclear structures. Vibrations stayed with him in his war-time projects when he studied the vibrations of larger structures, including airplanes. This may have been the reason that he never wanted to fly and never used air travel. When after the war he was interviewing for a job at Harwell, which might have involved classified work in the British nuclear program, he remarked on his German ancestry and expressed the hope that it would not prevent him from getting clearance. The irony of the situation was that the interviewer was Klaus Fuchs, a German who had participated in the Manhattan Project and turned out to be a spy for the Soviet Union.

Jahn was a quiet and modest man, very different from Edward Teller. He had a wide range of intellectual interests, including European literature, and was noted for his patient encouragement of his postgraduate students.

Afterlife

Today we can speak about Jahn–Teller “effects,” rather than just one effect, as they include some derivatives of the originally postulated effect, such as the pseudo-Jahn–Teller effect. There are monographs published about the Jahn–Teller effect and international conferences held regularly about it. The Jahn–Teller effect served as a starting point in

the quest for high-temperature superconductors by J. Georg Bednorz and K. Alex Müller at an IBM research laboratory in Switzerland. They made their discovery in 1986 and were awarded the Nobel Prize in Physics for 1987, one of the fastest awards ever made after a discovery in the history of the Nobel Prizes. The laureates paid ample tribute to the Jahn–Teller effect in their joint Nobel lecture and illustrated it in two attractive figures [2].

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References

1. Jahn HA, Teller E (1937) Proc Roy Soc Lond A 161:220–235
2. Bednorz JG, Müller KA (1993) Nobel lectures physics 1981–1990. World Scientific, Singapore, pp 424–457
3. Born M, Oppenheimer R (1927) Annalen der Physik 84:457–484
4. Herzberg G (1985) Annu Rev Phys Chem 36:1–30, 10
5. Herzberg G, Teller E (1933) Z Phys Chem 21:410
6. Renner R (1934) Z Phys 92:172
7. Dressler K, Ramsay DA (1959) Phil Trans Roy Soc Lond 251A:553–602
8. Hargittai I, Hargittai M (2008) Struct Chem 19:181–184
9. Hargittai M, Hargittai I (2009) Symmetry through the eyes of a chemist, 3rd edn. Springer, USA, pp 305–306
10. Hettema H (2000) Quantum chemistry: classic scientific papers. World Scientific, Singapore, pp 61–62
11. Hargittai M (2009) Struct Chem 20:21–30
12. Renner R (1933) “Lebenslauf des cand phys,” Göttingen, 1. XI. 1933, in the collection of Universitätsarchiv Göttingen
13. Landsberg PT (1980) Bull Lond Math Soc 12:383–386