An investigation with respect to the possible fabrication of research data reported in the thesis ETH No 13629 and in the papers Journal of Chemical Physics 112 (2000) 2575 and 113 (2000) 561

conducted by an investigation committee consisting of:

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upon request by the executive board of the ETH Zürich

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1. Introduction

Towards the end of the year 2008 two professors at the ETH, Prof. Peter Chen and Prof. Frédéric Merkt, who had been trying to remeasure and reproduce experimental data that had been produced in the research group of Peter Chen during the years 1999 and 2000, befell the suspicion that data published in the paper JCP 113 (2000) 561, authors Thomas Gilbert, Ingo Fischer and Peter Chen, had been fabricated. After having informed his former co-workers Thomas Gilbert and Ingo Fischer, on January 1, 2009 Peter Chen put a request to the executive board of the ETH Zürich (further Schulleitung) to stage an independent investigation into the possibility of the occurrence of scientific misconduct in his research group. In its sessions of January 20 and February 3, 2009, the Schulleitung decided to install an investigation committee with the task to investigate the question whether in relation to the publication JCP 113 (2000) 561 a case of scientific misconduct has occurred at the ETH. The committee consisted of

- Prof. Andreas Pfaltz, organic chemist at the University of Basel, acting as chair,
- Prof. Wilfred F. van Gunsteren, theoretical physicist at the Laboratory of Physical Chemistry of the ETH Zürich and vice-chair of the Department of Chemistry and Applied Biosciences, acting as coordinator.
- Prof. Martin Quack, physical chemist, spectroscopist and kineticist, at the Laboratory of Physical Chemistry of the ETH Zürich,
- Prof. Walter Thiel, theoretical chemist and director at the Max-Planck Institut für Kohlenforschung in Mülheim an der Ruhr, Germany, and
- Prof. Douwe A. Wiersma, physical chemist, spectroscopist, retired professor and dean of the Faculty of Natural Sciences of the University of Groningen, The Netherlands.

After study of the available data, the investigation committee (further IC) could fix April 27, 2009 as date for interviewing the three authors of the mentioned paper and two additional experts that were involved in the effort to remeasure and reproduce the original data, Dr. Andreas Bach, research assistant

(Oberassistent) in the research group of Peter Chen and Prof. Frédéric Merkt of the Laboratory of Physical Chemistry at the ETH. The answers by the persons interviewed to the questions by the committee members have been taken to protocol. A summary of the activities of the IC can be found in Appendix 1 to this report.

In the course of the investigation, it turned out that apart from the data on the allyl radical (C_3H_5) published in JCP 113 (2000) 561, also data on the propargyl radical (C_3H_3), published in JCP 112 (2000) 2575, show inconsistencies indicative of fraud. These data have also been reported in chapter 2 of the PhD thesis of Thomas Gilbert, "Hochauflösende Photoelektronenspektroskopie und Dissoziationsdynamik von Kohlenwasserstoffradikalen", ETH thesis No 13629. The PhD examination took place on 14 April 2000, with Prof. Peter Chen as referent, Prof. Frédéric Merkt and Dr. Ingo Fischer as co-referents, and Prof. Roel Prins as chair of the examination committee in his capacity of chairman of the Department of Chemistry of the ETH. The IC decided to make these three documents the subject of its investigation into possible misconduct. Other publications that may partially be based on the investigated data, such as Faraday Discussions 115 (2000) 17 and J. Phys. Chem. A106 (2002) 4291, are left out of consideration.

Appendix 2 contains copies of the two JCP papers and the thesis (2.1: propargyl; 2.2: allyl; 2.3: PhD thesis). We shall denote these documents JCP1, JCP2 and thesis. In Appendix 3 we include an internal report by Robert Pfab, a summer exchange student from Cambridge University, who did measurements on both molecules in the Chen research group during the summer months of 1999. As it became clear that the originally published data on the allyl radical could not be reproduced experimentally, Dr. Andreas Bach conducted an analysis of the various reported spectra. His two reports (December 2008 and March 2009) are included in Appendix 4.1 and 4.2, respectively. Regarding the allyl data, a retraction of JCP 113 (2000) 561 has been submitted to, accepted by, and published in JCP in 2009, see Appendix 5. A manuscript describing new measurements of the ionisation energy and

photoionisation of the allyl radical by M. Gasser, A. Bach and P. Chen of the Chen research group and A. M. Schulenburg, P. M. Dietiker and F. Merkt of the Merkt research group has been submitted to, accepted by, and published in JCP in 2009. The submitted version is contained in Appendix 6. We denote this manuscript as JCP3. The published version differs slightly from the submitted one. The differences are not relevant to this report. Regarding the propargyl data, efforts to reproduce these were started early 2009 after the suspicion of fabrication of the allyl data had come up at the end of 2008.

In the following, we shall first briefly describe in Section 2 the type of experiments that produced the suspicious data. In Section 3 we reconstruct and sketch the course of events since the measurements were carried out (1999, 2000). In Section 4 we discuss the apparent inconsistencies and irregularities in the reported and published data. In Section 5 we list the possible explanations for their occurrence. It is the unequivocal conclusion of the five IC members, the two experts (denoted as AB and FM) and the three authors of the papers (denoted as PC, IF and TG) that some data that were reported must have been fabricated. In Section 6 we consider the various responsibilities of the three authors of the data, PC, IF and TG. Section 7 contains our conclusions and recommendations to the Schulleitung of the ETH.

2. The types of experiments and data

The experiments that were used to obtain the experimental data in JCP1, JCP2 and chapter 2 of the thesis are so-called zero kinetic energy (ZEKE) photoelectron spectroscopic experiments, which make use of pulsed electric field ionisation of high-lying Rydberg states of molecules in the gas phase. A laser is tuned across the ionisation thresholds and an electron signal appears in the detector whenever the laser wavelength is in resonance with molecular Rydberg states characterised by state numbers n≈200, approaching the ionic states. Different techniques can be used to bring the molecule into a highlying excited state (i) resonantly enhanced multiphoton excitation, (ii) single photon excitation using a tunable vacuum ultraviolet (VUV) laser, and (iii) nonresonant two-photon excitation. Obtaining ZEKE spectra of radicals is highly non-trivial due to the difficulty of generating these reactive species cleanly and at high number density and due to the generally short lifetimes of excited electronic states of radicals. The radicals can be generated by supersonic jet flash pyrolysis and detected by mass spectrometry. The experimental set-up used to generate the data that are investigated is described in JCP1 and JCP2 and in chapter 2 of the thesis. Fig. 2.2.2 of the latter also illustrates various ZEKE excitation schemes, a non-resonant [1+1] process, a resonant [2+1'] process and a resonant [1+1'] process. Various lasers were used.

The photoelectron current measured by the detector is registered as function of the laser wavelength. The data are calibrated by comparison to known spectra of simple molecules. If data are measured in different experiments, e.g. covering different wavelength ranges, a combined (overall) spectrum is obtained by connecting partial spectra so that wavelength ranges recorded in more than one partial spectrum match. Thus first one obtains *raw data*, output from the detector and scanning laser, which are then combined into spectra. This is done using a software package, e.g. Excel from Microsoft Inc. or OriginPro from OriginLab Inc. In the case considered here OriginPro was used and the processed data were kept as so-called *Origin files*. Laboratory notebooks are used to register the various experimental runs, their parameter settings, the names of the files with the raw data and of those of the Origin

data. The latter were used to produce the figures in JCP1, JCP2 and the thesis.

3. Reconstruction of the course of events

In this section we roughly sketch the course of events that is relevant to this case.

- 2nd half 1998, early 1999: ZEKE experiments on (mostly non-radical) test molecules, NO, CS₂, fluorobenzene and toluene, are carried out in the Chen group by IF, TG and Thomas Grebner. Toluene served as reference for energy calibration in later experiments.
- Spring 1999: first ZEKE experiments in the Chen group that yield spectra of a radical, allyl, although of rather low resolution. They are carried out by TG. IF is Oberassistent in the Chen group. Thomas Grebner leaves the ETH (records of the personnel office have 31/3/1999 as exit date).
- Summer 1999: An exchange student from Cambridge (UK), Robert Pfab, stays four months (June-September) in the Chen group and performs ZEKE experiments mainly on the allyl radical and initial ones on the propargyl radical. According to IF, TG repeated and extended the propargyl experiments during August-September.
- 20 October 1999: A manuscript on the ZEKE spectrum of the propargyl radical is submitted to JCP, authors TG, R. Pfab, IF, PC. It is published in February 2000 (see JCP1).
- November 1999-January 2000: Further ZEKE experiments on allyl are carried out by TG. IF states that he was occasionally present during the measurements.
- 25 February 2000: A manuscript on the ZEKE spectrum of the allyl radical is submitted to JCP, authors TG, IF and PC. It is published in July 2000 (see JCP2). The first adiabatic ionisation energy (denoted by IE in this report), i.e. the energy difference between the ground state of

the allyl cation ($C_3H_5^+$) and the ground state of the allyl radical (C_3H_5) is reported to be 65762 cm⁻¹ or 8.153 eV with an estimated error of ±5 cm⁻¹. In the scientific literature, it is customary to report ionisation energies either as proportional to wave numbers in units of cm⁻¹ or as energies in eV, in which case one also uses the term ionisation potential; 1 eV = 8065.544 cm⁻¹.

- 14 April 2000: PhD examination of TG with PC as referent and IF and FM as co-referents.
- Summer 2000: TG leaves the ETH (records of the personnel office have 30/6/2000 as exit date).
- November 2000: Wu et al. of the National University of Taiwan, Taipei, publish (JCP 113 (2000) 7286) an IE of 8.138 (2) eV for allyl derived by Rydberg series extrapolation. This is in disagreement with the JCP2 data of the Chen group.
- Late 2000, early 2001: In order to elucidate the discrepancy, IF looks for the laboratory notebooks and the raw data files of TG, but cannot find them. After contacting TG, IF searches for them at the indicated locations but cannot find them.
- March 2001: IF leaves the ETH to take up a professorship at the University of Würzburg, Germany.
- Summer 2001: IF has information exchange and discussions about the source of the disagreement with Prof. Y. T. Chen of the Taipei group, who submitted a manuscript on the allyl radical on 28/6/2001 to JCP. It was accepted in December 2001 and published in March 2002, JCP 116 (2002) 4162. The IE was reported to be 8.133 (1) eV. During this summer, the Department of Chemistry including the Chen group moved from the CHN building downtown to the HCI building on the Hönggerberg.

- October 2002: In an attempt to resolve the discrepancy IF measures photoionisation and photoelectron spectra using synchrotron radiation at a light source in Orsay, France. The IE is determined to be 8.13 (1) eV in agreement with the value found by the Taipei group. The data are published in JCP 118 (2003) 9077 and Int. J. Mass Spectrom. 261 (2007) 227.
- Early 2003: Since the discrepancy is still not resolved, IF contacts TG in order to discuss possibilities to check the energy calibration of the old spectra, which turned out to be impossible because of the missing laboratory notebooks and raw data files. TG reports that he cannot find the notebooks at his home.
- April 2003: IF informs the Taipei group of his new results that agree with their earlier ones.
- Summer 2003: IF and PC discuss various explanations for the discrepancy, e.g. effects of rotational states that are populated due to insufficient cooling. Attempts by IF to repeat the original two-photon experiments in Würzburg fail.
- Early 2007: Prof. C. Y. Ng of the University of California in Davis informs IF about his VUV-ZEKE measurements on allyl, which yield an IE that disagrees with that of the Chen group (JCP2). The work of the Davis group is published in May 2007 (JCP 126 (2007) 171101) and reports an IE of 8.13146 (25) eV.
- March 2007: IF and PC discuss possible flaws in the interpretations of the Davis group, which has used experimental methodologies developed by FM. AB of the Chen group is asked by PC to check the various issues and to repeat the allyl experiment.

- September 2007: The new spectra by AB indicate that there is a problem beyond energy calibration. The old data are inconsistent with the new ones. FM is asked to carry out experiments in his laboratory using a different excitation scheme.
- December 2007: Planning of a comprehensive experimental study by
 AB, FM and PC to resolve all known discrepancies.
- Summer 2008: The measurements by AB and FM show that some intermediate states of allyl must be reassigned. This partly explains the discrepancy in IE values. However, these measurements also show that the old data are inconsistent: on the basis of the old (faulty) assignment they should have yielded different IE values instead of identical ones (in JCP2).
- December 2008: Close inspection of the old data for allyl shows various inconsistencies and irregularities: noise in spectra that is exactly identical between different parts of the spectra, the value of the IE obtained from the C-state, and an unusual scaling of the x-axis (energy) in some spectra. Comparison with the new data shows that some peaks in the old spectrum are absent in the new spectrum measured by AB and FM, see the report by AB of 31/12/08, Appendix 4.1. Together with the missing laboratory notebooks and raw data files these findings hint at fabrication of data.
- January 2009: PC requests an investigation into possible fraud from the Schulleitung, which composes an investigation committee.
- February 2009: The manuscript with the new data by Gasser et al. (see Appendix 6) is submitted to JCP. The IE of allyl is found to be 8.13088 (24) eV for one-photon excitation and 8.13103 (99) eV for resonant two-photon excitation, i.e. 65580.1 (20) cm⁻¹ and 65581.3 (80) cm⁻¹, respectively.

- March 2009: A retraction of JCP 113 (2000) 561 (JCP2), which contains the allyl data, is submitted to JCP (Appendix 5) and accepted for publication. AB sends an addendum to his report of 31/12/08 to the IC (Appendix 4.2). It contains a comparison through enlargement of allyl versus propargyl spectra originating from the Pfab report (Appendix 3, Fig. 3) and from JCP1 (Appendix 2.1, Fig. 1), respectively, which show large sections of identical noise.
- 27 April 2009: The investigation committee conducts interviews with AB, FM, PC, IF and TG.
- 17 June 2009: A draft report by the IC is sent to PC, IF and TG with a request for suggestions for improvements of the report. Such suggestions are received on 23/06/09 from IF, on 30/06/09 from PC, and on 12/07/09 from TG.
- 7 July 2009: The retraction of JCP2 and the manuscript JCP3 are published on-line in JCP, see JCP 131 (2009) 019903 and 014304, respectively.
- 10 July 2009: TG declines an invitation by the IC to hold a second hearing with him about the draft of the report.
- 15 July 2009: The definitive version of the report by the IC is sent to PC, IF and TG with a request for their comments to be included in Appendix 7.1-3 of the final report.
- August 2009: The investigation committee presents the final report of its investigation to the president and the Schulleitung of the ETH. A copy is sent to PC, IF and TG, and to the experts AB and FM.

4. Inconsistencies and irregularities in the data

The following data show inconsistencies and irregularities:

- Figs. 1 and 2 of JCP1,
- Figs. 2, 3 and 4 of JCP2,
- Figs. 2.4.8, 2.4.9, 2.5.5, 2.5.6, 2.5.8, 2.5.10 of the thesis.

The indicated figures of the two JCP papers appear also in the thesis:

- Fig. 1 of JCP1 corresponds to Fig. 2.4.8 of the thesis,
- Fig. 2 of JCP1 corresponds to Fig. 2.4.9 of the thesis,
- Fig. 2 of JCP2 corresponds to Fig. 2.5.5 of the thesis,
- Fig. 3 of JCP2 corresponds to Fig. 2.5.8 of the thesis,
- Fig. 4 of JCP2 corresponds to Fig. 2.5.10 of the thesis.

4.1. Recurrent noise in a spectrum

Close inspection of the figures shows recurrent noise patterns in Figs. 2.4.8-9, 2.5.5-6, 2.5.8 and 2.5.10 of the thesis and also in their counterparts Figs. 1 and 2 of JCP1 and Figs. 2-4 of JCP2. The numerical analysis of the noise patterns in Fig. 3 of JCP2 and Fig. 2.5.8 of the thesis containing allyl data by Bach in his report of 31/12/2008 (Appendix 4.1) shows that identical ranges of noise are present within a single spectrum and in different spectra. The same observation holds true for the spectra in Figs. 1 and 2 of JCP1 and Figs. 2.4.8-9 of the thesis. Last but not least the noise in the 390 – 393 nm range in the spectrum of the *allyl* radical in Fig. 3 of the Pfab report (Appendix 3) is identical to that in the spectrum for the *propargyl* radical in Fig. 1 of JCP1 (Fig. 2.4.8 of the thesis), see the report by AB of 4/3/2009 (Appendix 4.2).

4.2. Occurrence of non-standard scaling of the energy in a spectrum

Numerical analysis of the Origin data corresponding to parts of Fig. 3 of JCP2 (Fig. 2.5.8 of the thesis) shows that the data points are uniformly spaced along the x-axis, i.e. in energy, exactly 1.0 cm⁻¹ apart, at integral values of the energy unit cm⁻¹. This spacing is unusual, because according to PC up till recently all past and present lasers in his laboratory, including the ones used to measure the data presented in JCP1, JCP2 and the thesis, scan through an energy range by finite steps linearly in wavelength (which is inversely proportional to the energy or laser frequency), not linear in frequency. Some of the most recent lasers, e.g. some lasers used to measure data reported in JCP3, can make finite mechanical steps that are not linear in wavelength.

4.3. Peaks in the old spectrum that are absent in the new one

In Fig. 4 of JCP2 (Fig. 2.5.10 of the thesis) two peaks indicated as v_{12}^+ at 274 cm⁻¹ and v_9^+ at 612 cm⁻¹ are present in the [2+1] ZEKE spectrum obtained from the B0 $_0^0$ state. In the new measurements, Fig. 5 of Gasser et al. (Appendix 6), these peaks are clearly missing. See also the comparison in Fig. 4 of the report by AB of 31/12/2008 (Appendix 4.1).

4.4. Ionisation energy as determined from different intermediate states

The [2+1'] ZEKE spectrum from the BO_0^o state as presented in Fig. 4 of JCP2 (Fig. 2.5.10 of the thesis) yields an ionisation energy that is equal to that calculated from the [1+1'] ZEKE spectrum from the CO_0^o state as presented in Fig. 3 of JCP2 (Fig. 2.5.8 of the thesis). It is now known that the CO_0^o state has not been located correctly in JCP2 (see JCP3), and therefore it should have been impossible to observe ZEKE spectra (as reported in JCP2) that lead to an identical ionisation energy.

5. Possible explanations of inconsistencies and irregularities

After having analyzed the inconsistencies and irregularities described in Section 4, the IC has discussed possible causes.

Since a complete spectrum is often composed by merging spectra of limited wavelength range, an inadvertent copying of one wavelength range onto another might happen, which would lead to recurrent noise patterns.

However, the extent of the observed recurrences of noise patterns makes this explanation unlikely. The irregular pattern of the recurrences basically rules out faulty software as the culprit. It also rules out recurrent noise patterns originating from the power grid as a possible culprit. The only credible explanation is manipulation of the data, which, however, cannot be traced closer to its source because of the missing laboratory notebooks and raw data files regarding these experiments. We note in passing that according to PC and AB the laboratory notebooks of TG are the only ones missing from the Chen research group. We have verified the presence of laboratory notebooks of more than forty former PhD's and post-docs of the Chen research group. No laboratory notebooks of TG were present in the collection.

These missing original data also preclude an unequivocal explanation of the occurrence of a linear energy scale in some of the spectra. Again faulty software can be reasonably excluded to produce equidistant data points upon executing an inversion, which leaves copying or fabrication as the only plausible explanation.

Regarding the two indicated peaks, ν_{12}^+ and ν_9^+ , that are present in the old allyl spectrum but not in the new allyl spectrum, it was suggested by TG that they could at the time have resulted from impurities in the sample. However, such impurities should have been easily detected via the mass spectrometer considering the fact that the allyl radical is a very simple molecule (C_3H_5). A more likely explanation is that these peaks in the spectrum have been fabricated based on the interpretation of the experiments in combination with

theoretical knowledge at the time about the excitation mechanisms and the vibrational spectrum.

The IE's obtained via different excitation mechanisms and experiments were reported as being the same, but it is known in retrospect that the intermediate state in one of the experiments is not located at the originally assumed position. It is difficult to imagine how to obtain spectra (other than by fabrication) that yield the same IE when the required intermediate state is not present in one case.

Based on these observations and considerations the two experts interviewed (AB and FM), the three authors interviewed (PC, IF and TG) and all IC members agreed that fabrication of data must have occurred. The next question is who has done it.

The person who measured the data and had the easiest access to the data is TG. However, he explicitly denies having manipulated or fabricated the data. The measured raw data were kept on computers which were not password protected, which is common practice in science because different group members make use of the same measurement devices at different times. In principle, anyone with access to the laboratory could have manipulated the files. This includes a large group of people as pointed out explicitly by TG during the interview with the IC. However, due to the sophisticated character of the manipulations required, it is virtually impossible that anyone who does not have a thorough knowledge of the theory and spectroscopy of radicals and ZEKE experiments could have produced the inconsistencies and irregularities discussed above. Note in particular that considerable expertise was required to put the "wrong" peaks in the reported spectra (Sections 4.3 and 4.4) at plausible positions that were consistent with the theoretical and spectroscopic knowledge on allyl available at the time of the original experiments. The IC has considered all persons, who according to their knowledge could have manipulated the data, and their possible motivations.

IF and PC, both intending to continue their career in science, would have no motive to fabricate data. Their efforts to remeasure the data, thereby involving independent research colleagues, would be at odds with such an assumption. TG, when the point was discussed with the IC, also stated that he ruled out data manipulation by IF or PC. The exchange student Pfab was only four months in the laboratory and his report clearly hints at difficulties obtaining clean spectra. The other group member who had been involved in ZEKE experiments, post-doc Thomas Grebner, did leave the laboratory in spring 1999 (31/3/1999 according to data from the personnel office of the ETH). This leaves TG as the most likely culprit. According to himself and IF and PC, he did most measurements on his own. After getting him started with ZEKE experiments, IF was occasionally present when collecting data, and PC and IF generally saw data as presented by TG to them, e.g. at group meetings. What might have been a motivation for TG to manipulate data? Both, TG on the one hand and PC and IF on the other denied to have felt or exerted any mutual pressure to produce publishable data. One possible motive might be that TG felt under pressure to produce such results, if he had already considered to apply for jobs by the end of 1999 (before the final data on the allyl were obtained). In order to have sufficient data for a thesis and to avoid delay because of inconsistent data, good results would have had to be produced. After completing his PhD thesis work TG left chemical research.

It is the unequivocal opinion of the IC that TG is the only likely person to have manipulated and fabricated data published in JCP1, JCP2 and his PhD thesis. Any alternative to be considered would involve an unidentified person with a high level of technical knowledge in the field and high criminal energy and at the same time irrational, possibly mentally perturbed motivations. No such person could be possibly identified by the IC.

The IC has considered any possible omissions in the preparation of the present report. While TG agrees that data have been manipulated, he consistently denies to have contributed to this himself. In view of the obvious contradiction between this latter statement and the conclusions of the IC, the IC has offered TG the opportunity for an additional hearing and discussion

with the IC, where additional arguments or evidence could have been presented by TG to convince the IC of his case. TG has rejected this offer for an additional hearing.

6. Responsibilities regarding the fabrication of data

Given that fabrication of data has occurred in the research group of PC resulting in research publications and a PhD thesis that contain fabricated data, which are the responsibilities of the various persons and organisational units involved? Should the authors or their colleagues, the department or the Schulleitung have acted earlier than and differently from what they have done (see Section 3)?

Independently of the question who manipulated the data, TG bears full responsibility for the data contained in his thesis. If he did not manipulate the data himself – quod non according to the IC – he should have noticed – as the one who had done the measurements – the irregularities.

Independently of the question who manipulated the data, PC, IF and TG, being authors of the papers JCP1 and JCP2, bear full responsibility for their contents. The challenge to measure ZEKE spectra and adiabatic ionisation energies of allyl and propargyl was taken up by PC and IF, his right hand in his research group at the time. They devised the experiment and designed the equipment, which was home-made and custom-built for the experiment.

As soon as the data in JCP2 were questioned by other research groups, IF considered various explanations, discussed with the authors of papers reporting differing results, and set up experiments to solve the discrepancy with the means he could reasonably make available in his position at the University of Würzburg. IF was as Habilitand in the Chen group not directly responsible for the work of TG.

After the first emergence of discrepancies between the results of the Chen group with those of the Taipei group (published in 2000 and 2002), PC considered possible explanations with IF, but was not too worried because the discrepancies in IE were not very large and there were methodological doubts concerning the accuracy of the results from the Taipei group. He left it to IF to try to resolve the discrepancy using synchrotron radiation experiments. Only

after the research group at Davis reported (2007) the same discrepancies in IE using a high-resolution technique, was a remeasurement initiated and a considerable effort spent to clarify the situation. The involvement of an expert colleague (FM), apart from the current Oberassistent in the Chen group (AB), was an effective move to delineate the inconsistencies. Both, the new experiments in the Merkt group and the investigations and measurements by Andreas Bach (Appendix 4.1-2), made clear that a case of fabrication of data could have occurred. The next step of an independent investigation was properly taken.

In our opinion, both IF and PC have taken the appropriate steps to solve the inconsistencies and irregularities that have emerged over the course of time. Repeating the original measurements was difficult and also expensive. With the move of the Chen group to the Hönggerberg in 2001, the research focus changed away from ZEKE experiments, and the experimental ZEKE set-up was no longer operational. Because of the shift of the research focus, the inconsistencies in the old data were not noticed in the Chen group itself. Since not many research groups are active in this field, it took a long time (until 2007) before credible conflicting data were published that made a reinvestigation necessary which was then carried out with considerable investments in manpower and hardware.

In retrospect, one may ask why the recurring noise patterns in some spectra, being the most direct evidence of fabrication of data, were not noticed at the time of submission and review of the PhD thesis and the publications. One obvious reason is that spectroscopists mainly look at peaks, not at noise. Furthermore, one does not read a thesis, manuscript, or paper with the expectation of meeting fraud. Even the reviewers of the manuscripts JCP1 and JCP2 and the research groups that published the data differing from those by the Chen group did not notice (as far as known) the recurrence of noise. One cannot expect from co-referents at a thesis examination or a department conference to detect irregularities of the type discussed here.

As a consequence of containing flawed data, the publications reporting them should be (partially or completely) retracted. For the JCP2 paper this has been done. For the thesis and the JCP1 paper this is still to be done, which is a primary and urgent responsibility of the authors. In addition, the research colleagues of the authors of the papers have to be informed by them that these are based on fabricated data.

Finally, should any organisational measures be taken to avoid fabrication of data at the ETH? First of all, it is an illusion to think that fraud can be avoided by organisational means. The major correction mechanism, publication of research results followed by reproduction or confirmation by other research groups, still functions in science and is a deterrent to fraudulent minds. Second, a research climate in which double checking has a higher value than quick publication is of great importance to research of high quality and to the education of researchers of high integrity. We see no grounds to change the formal procedures to obtain a PhD degree or to publish research data at the ETH.

7. Conclusions and acknowledgements

Parts of the data published in JCP1, JCP2 and the thesis have been fabricated. This is the unequivocal conclusion of the IC, the two experts and three authors of the two papers and PhD thesis that were interviewed by the IC. The IC is of the opinion that TG is the only likely person to have manipulated and fabricated the data as discussed in this report.

As soon as the efforts by IF and PC to reproduce the propargyl data published in JCP1 yield a more complete picture of the extent of their irregularity or incorrectness, the authors of JCP1 must take appropriate steps (partial or full retraction), as has already been done with JCP2. The author of the PhD thesis must retract his thesis, which implies renouncing the Doctor title that was conferred to him based on his PhD thesis. It is the duty of the Schulleitung to see to it that these retractions are carried through in due time. PC has informed the IC that he wishes to appropriately inform his colleagues about this case of fabrication of data in his research group as soon as the report of the IC has been released to this end by the Schulleitung.

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