FRITZ HABER CENTER SYMPOSIUM IN MEMORY OF

Professor Victoria Buch, 1954-2009

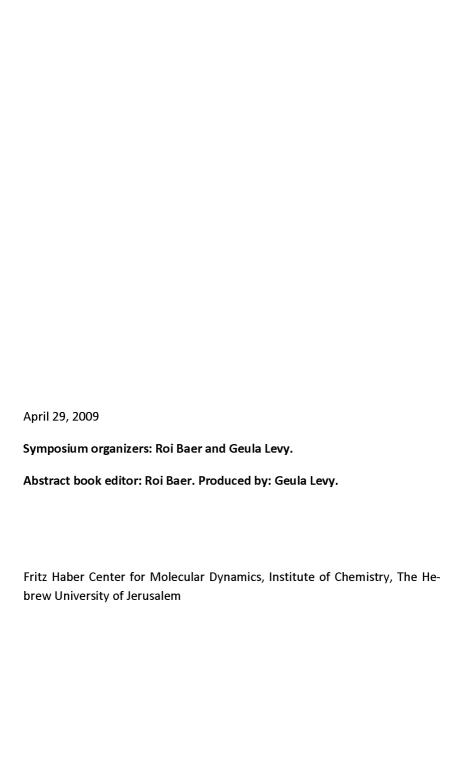


A pioneer in the theory of ice and water surface chemistry,

A brave human rights activist

May 10, 2010

Fritz Haber Center for Molecular Dynamics,
Institute of Chemistry, The Hebrew University of Jerusalem



$PROGRAM \ (\texttt{Chemistry Seminar Hall}, \texttt{Los Angeles Bldg.})$

08:45	R. Baer, Nina Mayorek	Welcome and Opening remarks	
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Chair: Noam A	gmon, The Hebrew Univer	sity Session 1		
09:00 - 09:40	R. Benny Gerber, The Hebrew University	A Passion for Science: Victoria Buch's Life in Research		
09:40 - 10:20	J. Paul Devlin, Oklahoma State Univ.	ULTRAFAST CLATHRATE-HYDRATE CRYSTALLIZATION FROM SUPER- COOLED NANODROPLETS		
10:20 - 11:00	N. Uras-Aytemiz, Suleyman Demirel Univ.	COMPETITIVE ADSORPTION OF HNO ₃ & HCL IN WATER CLUSTERS & ICE		
11:00 - 11:30	Caffeine Break			
Chair: Dan Huppert, Tel Aviv University Session 2				
11:30 - 12:10	Joanna Sadlej, University of Warsaw	CHARACTERISATION OF DIHYDROGEN- BONDED D-HH-A COMPLEXES		
12:10 - 12:50	Avinoam Ben- Shaul, The Hebrew University	COMPACTNESS, FOLDING AND AP- PARENT CIRCULARIZATION OF SSRNA		
12:50 - 14:00	Lunch			
Chair: Audrey Del Hammerich, Univ. of Illinois at Chicago Session 3				
14:00 - 14:40	Michele Parrinello, ETH Zurich, Switzerland	Advanced sampling methods		
14:40 - 15:20	Matania Ben-Artzi, The Hebrew University	SIMULATION OF REACTING FLOWS WITH STIFF SOURCES		
15:20 - 15:50	Caffeine Break			
Chair: Ehud Pines, Ben-Gurion University of the Negev Session 4				
15:50 - 16:30	Erio Tosatti, SISSA, Trieste, Italy	ICE AND VICTORIA BUCH: A COLD SURFACE AND A WARM HEART		
16:30 - 17:10	Pavel Jungwirth, Academy Sciences	HYDRONIUM AND HYDROXIDE AT THE		

THE INTENSITY OF THREE LIFE SPANS

Dassi Elber, 26/6/09

During the Shiva for my mother, Victoria Buch, my aunt Nina Mayorek and I agreed upon one aspect of Victoria that is indisputable: her untimely death notwithstanding, my mother lived her life with the intensity of three life spans.

My mother gave her heart and soul to every activity she was involved in, be it personal, political or academic. For example,



during my teenage years, my high school invited various lecturers to speak about chemistry, physics, astronomy, and other topics within the natural sciences. Most of the lecturers tended to lull the students to sleep with dry speeches and elaborate taxonomy. My mother, however, dedicated an entire week to constructing a beautiful PowerPoint presentation with dazzling pictures of supernovas, falling stars, and black holes. In simple, colloquial language, she held the attention of an entire classroom of high school teenagers, even eliciting bursts of laughter as she joked with them about the principles of astrophysics. After the lecture was over, and my co-students burst in applause, she asked me with typical modesty, "I didn't embarrass myself before your friends, did I?"

In the final weeks of her life, my mother still refused to relinquish her goals in face of the illness that afflicted her. Barely three weeks before her death, while heavily medicated, she insisted on holding an academic conference in our house. Victoria collected herself, fought away the effects of her medica-

tion, sat in front of her computer and invited over her two postdoctoral students and her colleague, Paul Devlin. She then supervised the meeting, formulated scientific ideas, and engaged in active academic discourse for several hours straight. A week before her death, she finished the article that her group was working on.

The best way to honor my mother's memory, I believe, is to live as she lived, with absolute loyalty and dedication to those things in life that were truly dear to her. May we all have the insight, the strength and the conviction to do so.

A Passion for Science: Victoria Buch's Life in Research

R.Benny Gerber, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, the Hebrew University of Jerusalem

Abstract: I was fortunate to have been the advisor of Victoria Buch for her Ph.D., and since then was greatly influenced by her research, ideas and approach to science.

In this lecture, I will discuss the evolution of Victoria as a scientist, from the early years as a research student up to her development into an international leader in her field, and to the intensive, stimulating research she has pursued until the very last days of her life, when she was gravely ill.

I will mention research highlights, key accomplishments and results from different stages of Victoria's career. I will also discuss in some detail the important lessons I learned from a rewarding and successful last joint research project I have had with Victoria, towards the end of her days; how uncompromising and determined she was in her pursuit of science; her ability to follow new directions and ideas under the most trying circumstances.

I will present the view that Victoria's life and approach to research can be a source of inspiration to our young students.

I owe so much to Victoria Buch

I owe so much to Victoria Buch, and have learned so much from her as a scientist and as a person, that I am naturally flooded by memories from the many years of working and interacting with her. My thoughts right now are dominated by one recent experience. A few days ago, I visited Victoria at her deathbed. She found time and strength to see me, by sacrificing some of the few precious hours in which she was not sedated by morphine. We both knew this was a farewell visit, though we did not say this. Victoria said nothing of her suffering, which was terrible. Victoria spoke of science and of interesting research problems. She outlined very nice ideas, and expressed a vision for her research field. She was going to do whatever possible to complete projects she began, and was hopeful that they will be published. She knew the situation, and was prepared to suffer just to communicate for the future ideas that are important. This is a real Victory of commitment to science and to research over illness. Quite apart from the courage, in that discussion Victoria had the sharpness of mind and brilliance of argument characteristic of her. Victoria's ideas, research approaches and passion for science will be with me as long as I work and live. Her ideas will influence my work also in the future, and I think this is correct for a large group of scientists who new her. I am very fortunate that I had Victoria Buch as my student, then my friend and my colleague. – Benny Gerber

ULTRAFAST CLATHRATE-HYDRATE CRYSTALLIZA-TION FROM SUPERCOOLED NANODROPLETS

J. Paul Devlin, Dept. of Chemistry, Oklahoma State University, Stillwater, OK 74075

Abstract: I will briefly review the 20 years of collaborative research with Victoria and then present of our most recent results from clathrate-hydrate research. This is an extension of the earlier research which also dealt primarily with water-rich solid-state systems ... ice, the ice surface, solvation of adsorbates on ice, reactive adsorbates on ice, acid hydrates, ammonia hydrates, acid etherates, ice defect mobility and finally clathrate hydrates (CHs). One of the most vital properties of CHs is the rate at which they form from ice or aqueous solutions, or undergo transformations to related structures through gain, loss or replacement of guest molecules. It has been established that these rates are often greatly accelerated when one guest species is inclined to form a hydrogen bond with the host lattice water molecules [1]. Studies of these accelerated rates, that have previously been at cryogenic temperatures ranging from 100 to ~160 K, suggest that quite phenomenal rates should be observed at higher temperatures; e.g., 200 K. Here, a method of testing rates of formation of CHs at ~200 K is described and results detailed for several simple ether as well as mixed ether - smallmolecule CHs. Complete conversion of all available water to CHs on a millisecond timescale has been observed for numerous guest combinations; confirmation that phenomenal rates are realized. CH formation is observed by FTIR spectroscopy as temperatures of warm vapor mixtures drop rapidly to ~100 K in a cold condensation cell. That CH formation completely overrides ice nucleation and crystallization is indicative of the rapidity of the process.

[1] V. Buch, J. P. Devlin, I. A. Monreal, B. Jagoda-Cwiklik, N. Uras-Aytemiz and L. Cwiklik, Phys. Chem. Chem. Phys. (A Perspective) 11, 10245 (2009).

MODERN DAY HEROINE

Surely many of us recognize Victoria Buch as a modern day heroine. It is an honest view of this wonderful woman who had such a natural inclination to sacrifice time, energy, resources and her own security to work with great determination and obstinacy for justice where she saw injustice. It is no exaggeration to say she put her life on the line for a cause, as those suffering injustice have been a target of hate. She surely lived the dictum "if you seek peace, work for justice". I have often



Left to right: Victoria, Paul, Nevin (Turkey, 2004).

thought and sometimes expressed the idea that someone should write a book about all aspects of her life, but with particular emphasis on her devotion and actions for justice and peace. The book would, of course, have parallel threads for Victoria and her sister Nina, both of whom have demonstrated so well the power and personal strengths of the modern dedicated woman. The lives of such extraordinary people give meaning and comfort to the rest of us. I am exceedingly fortunate to have been gifted with significant time with Victoria, both in a personal and professional sense, and never ceased to be amazed by the varied achievements of this tremendously caring person with a brilliant mind. - Paul Devlin

THE INCIDENT WITH VICTOR BUCH

Early times... 1988. My group had been working on defect mobilities in ice near 100 K for about 8 years when V. Buch submitted a paper describing a computational model/result for water vapor condensing to amorphous ice at ~100 K. I reviewed it for JCP, liked it, approved it but suggested that he might want to apply his computational approach to the structure and motion of defects in ice. In the author's response to my suggestion, I learned it was Victoria Buch, and that my suggested computation was a difficult one that would have to wait for faster computers. She (with Natasha) successfully addressed the defect issue about 15 years later... and again more recently with respect to the ice surface.

HIKING WITH VICTORIA

We all know that Victoria loved to hike and talk (science) ... not truly hike in the Middle-European, Udo-Buck sense; more of a Mediterranean derivative. One afternoon, from Lugano, we traveled north a bit and climbed a steep hill. My feet were hurting badly, as I had not brought the right shoes from the States.



Hiking the Newfoundland coast near St. Johns. Summer, 2002.

Coming down we became engaged in the question of the nature of the vapor over HCl acid hydrates... in particular when the mono- and the dehydrate were present together in equilibrium. Soon, in an attempt to answer using the Phase Rule, our discussion became heated... as were my feet. As we neared the bottom Victoria suddenly realized I was right. Almost unheard of and very upsetting ... but my feet stopped hurting. She retained that moment with chagrin and humor. - Paul Devlin

ICE AND VICTORIA BUCH: A COLD SURFACE AND A WARM HEART

Erio Tosatti, SISSA, ICTP, and CNR/INFM Democritos, Trieste, Italy

Abstract: Victoria Buch, who knew so much about ice and hydrogen bonds, was intrigued and fascinated by the possible physical states of the ice surface.

She knew on one hand that it was only reasonable to expect the proton disorder of bulk ice to persist at the surface. She also felt on the other hand, or hoped, that the surface energetics should favor some new type of surface proton order, absent in bulk ice.

To pursue this fragile dream, she stole time away from both her heartier physico-chemical studies and her warm-hearted generous political battles within Israel, to collaborate with a surface theorist, whom she met by chance in Michele Parrinello's lab one summer in Lugano -- me.

Me, who would contribute nothing more than some generic wisdom, and no actual hard calculations. Her own simulations, both Molecular Dynamics and Monte Carlo, eventually showed that in the cold ice surface not only the oxygen atoms will stay put and crystalline up until some 180 K, but at low enough temperatures the protons too would order -- and that in spite of proton disorder in the underlying bulk! My own job ended up being the mere recognition that her identified surface order, 2x1 stripes formed by rows of "dangling hydrogens" and "dangling oxygens" (the same as an old suggestion by Fletcher) could finally make sense of some unexplained he-

lium scattering data published a decade earlier in Goettingen. As it also turned out, Victoria's American collaborators, Mary Shultz her group, had sum frequency data that lent some additional support to the idea.

During her stay in Trieste in October 2007 we discussed a lot how and where to publish. We hesitantly decided to try prestigious PNAS, and I started contacts with Steven Berry, who was indeed very constructive; and then Victoria left back to Jerusalem.

It was at this point that I was suddenly reached by Victoria's fatal phone call asking me to look after the work and the paper, for she could help no more. Eventually, our joint paper on the ice surface was published [1], fulfilling at least part of her dream. Victoria and I were still collaborating, and spending hours on the phone at that, during the following year -- she would say that physics had a therapeutic effect on her. She very much wanted to find out how fragile or robust the ordered surface striped phase would be against temperature. My own Landau theory and universality says there should be a first order transition between 2x1 stripes and thermal disorder, at some unknown temperature. Her preliminary model Monte Carlo study found precisely such a transition around 60 K. While we must now wait for some data or for newer, less tentative calculations to follow up on Victoria's, 60 K remains our best estimate for the "Buch transition" temperature between 2x1 striped order and proton disorder at the surface of hexagonal ice.

[1] "Proton order in the ice crystal surface, Buch V, Groenzin H, Lit I, et al., PNAS, 105, 5969 (2008).

COMPACTNESS, FOLDING AND APPARENT CIRCULA-RIZATION OF SSRNA

A. Ben-Shaul*, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, the Hebrew University of Jerusalem

Abstract: Due to partial matching of its bases single stranded (ss)RNA folds on itself into branched structures resembling composed of short double stranded duplexes connected by flexible loops. Using the "maximum ladder distance" $\langle M\!LD \rangle$ as a measure of RNA size we show that viral RNAs are consistently more compact than random sequences of the same length and base composition. They are also smaller than natural, non-viral, ssRNAs, suggesting that viral RNAs are more compact owing to the evolutionary pressure to facilitate their packaging into small rigid protein capsids. We found that the average $\langle M\!LD \rangle$ s of large non-viral ssRNAs scale as $\langle MLD \rangle \sim N^{0.7}$, where N is the number of nucleotides, and by mapping the secondary structures onto a linear polymer model we argue that their radii of gyration, $R_{\rm g}$, vary as $R_{\rm g} \sim \left< MLD \right>^{1/2} \sim N^{0.35}$. This may be compared to a randomly branched polymer, where $R_{_{\rm g}} \sim N^{0.25}$. Recent Cryo-Tem measurements and molecular dynamics simulations of model RNAs appear to support this difference. We shall also present an approximate, "sequential", folding model of ssRNA, which explains in simple terms why certain generic properties of its secondary structure, such as the average duplex length and the average base pairing probabilities are independent of N. The quantitative predictions of the model compare very well with those of more detailed numerical procedures. Finally, we shall explain why the secondary structures of linear and covalently-circularized RNAs are practically identical. Then, using elementary combinatorial and graph theory arguments we calculate another generic property of ssRNAs -- namely, the proximity of their 3' and 5' ends, and show that the end-to-end distance is small and independent of N.

* Work in collaboration with W. M. Gelbart , A. Yoffe, P. Prinsen, A. Gopal, L. T. Fang, and C. Knobler, all from UCLA.

HYDRONIUM AND HYDROXIDE AT THE SURFACE OF WATER

Pavel Jungwirth, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, 16610 Prague 6, Czech Republic

Abstract: Autoionization (autolysis) of water which gives rise to its pH is one of the key properties of aqueous systems. Surfaces of water and aqueous electrolytes solutions are traditionally viewed as devoid of inorganic ions, however, recent molecular simulations and spectroscopic experiments show

the presence of certain ions including hydronium in the top-most layer. This raises the question about what is the ionic composition of the surface of neat water. Microscopic simulations and measurements with atomistic resolution show that water surface is weakly positively charged due to a stronger propensity of hydronium than hydroxide for the



Telluride 2008. with Pavel Junwirth

surface. In contrast, macroscopic experiments, such as zeta potential and titration measurements, indicate a negatively charged water surface interpreted in terms of strong preferential adsorption of OH-. Here we present recent simulations and experiments characterizing autoionization at the

surface of liquid water and ice crystals and at the water/oil interface in an attempt to resolve the existing controversy.

This project started as collaboration with Victoria Buch during her sabbatical stay in Prague in winter 2007.

VICTORIA THE SKIER

Viki was a great and dedicated scientist and I should probably recall here one of the many inspiring occasions when we were doing serious science together.

But I cannot resist the temptation to tell a less serious story. During the years we have known each other we have done quite a bit of "after school" activities including going to mountains which we both enjoyed a lot. When Viki spent part of her last sabbatical with me in Prague in winter 2007 she joint us for a week of skiing in the Orlicke mountains in north Bohemia. We are a family of skiing addicts, so my idea was that I will serve as Viki's personal coach, passing part of the white powder addiction to her.

Well, we got the skies, got to the slope, I started my "training program" ... and it was a disaster. I did not quite realize that last time Viki skied was before she left Poland in 1968 and the progress was thus slower than I expected. Be a professional, I said to myself and with infinite patience and buckets of good spirit (Yes, we can!) I continued the skiing lesson. Until Viki looked at me with the piercing look she gave me several times before when I was running on her nerves and said: "Go f... yourself, Pavel, I can do this myself." And that's what we both did and by the end of the week Viki taught herself to turn elegantly and stop decently. I mean, she was not ready to go for international competitions but she was going down (mostly) without falling and was enjoying herself. Viki, I will miss your lessons on stubborness in the best sense of the word. And most of all, I will miss your piercing look.

- Pavel Jungwirth

CHARACTERISATION OF DIHYDROGEN-BONDED D-H...H-A COMPLEXES ON THE BASIS OF SPECTROSCOPIC PARAMETERS

Joanna Sadlej, Faculty of Chemistry, University of Warsaw, Poland

Abstract: The properties of dihydrogen-bonded dimers with the LiH and BeH₂ molecules as a proton acceptor were calculated by MP2 and CCSD(T) methods. The structural, energetic and spectroscopic parameters are presented and analyzed in terms of their possible correlation with the interaction energy and the intermolecular H...H separation. The symmetry-adapted perturbation theory (SAPT) calculations were performed to gain more insight into the nature of the H...H interaction. The complexation - induced changes in vibration frequencies and in proton shielding NMR constants show a relationship with the interaction energy. The values of some spin-spin coupling constants correlate well with the interaction energy and with the intermolecular distance. It was found - there is no sharp boundary between the dihydrogen-bonded complexes (DHB) classified as hydrogen bonded and van der Waals systems.

VICTORIA BUCH BY J. SADLEJ, ORBITAL, 1,(2010),63-64

The last professor Victoria Buch publication lies on my desk in front of me: Clathrate hydrates with hydrogen-bonding guests (PCCP, 2009, 11, 10245-10265). On the first page, her photo and the photograph of professor Paul Devlin, her long-time collaborator spectroscopist; the next pages show two young PhDs from Kraków who were working under the leadership of professor Buch. She had finished the article mentioned above and sent it for publication a week before her death, as she was fighting her fatal disease. The news about her early death (she died on the 21st of June 2009 at the age of 55) spread quickly all over the world. The next day, on the Hebrew University website numerous recollections and words of gratitude appeared from

people who were lucky to know Victoria and those who could work with her, others who were her friends or from far away could observe her activity. After all, she was so active in so many fields.

Victoria completed her chemistry studies in 1979; she obtained her PhD degree in the area of theoretical physical chemistry in 1984. She worked under professor R. B. Gerber at the Hebrew University of Jerusalem. Then

she joined professor A. Dalgarno's team at Harvard-Smithsonian Centre for Astrophysics and after two years she joined the Department of Chemistry at University of Illinois at Chicago. In 1992 she came back to Jerusalem, becoming associate professor (1995) and then full professor (2000). Victoria was invited to give lectures at numerous conferences including Gordon meetings in the USA. She was the co-organizer of conferences in

Victoria and Joanna (Zawrat, 1997)

Telluride, USA, and a Faraday Discussion (number 141). She has authored over 130 scientific papers, some published in the most

prestigious journals (Nature, Proc. Nat. Acad. Sci. US, Phys. Rev. Letters and J. Chem. Phys.). She is the co-editor of the book "Water in Confining Geometries" (Springer, Berlin, 2003).

Real scientists resemble creative artists: to them, work on scientific problems is a calling. They are totally immersed in it engaging their intellect, their heart and soul. That is their true life; that's the way they have chosen - work is an absolute necessity for them. When I met Victoria, she told me about the new Diffusion Monte Carlo method she developed for investigating the structure and spectroscopy of ice, and the absorption of gases on ice surfaces. This brought her close to her previous interests e.g. atmospheric chemistry and astrophysics. Those were "fairy tale" stories. At that time, she felt distinctively the necessity to establish close cooperation with spectroscopists - experimentalists. Very soon after, the experimental research of professor Udo Buck from Göttingen enabled her plans, concerning water, the most mysterious and unusual substance in nature, come to life. Later, experimental work of professor J. Paul Devlin concerning the IR spectroscopy of various adsorbates on ice allowed Victoria and Devlin to establish a theoretical-experimental cooperation connected (among other things) to the ozone hole or to the creation of stormy clouds. Victoria was ever so enthusiastic and passionate, always on the lookout for new areas of activity, open to worldwide scientific problems. She visited the Faculty of Chemistry at Warsaw University several times over the past fifteen years.

The world cannot be narrowed down to only scientific reality. One can be creative also in other life areas. "I came to Israel 40 years ago" – it is the quotation from Victoria Buch's text published on January 4, 2009 in *Occupation Magazine*. The Buch's left Poland in 1968 when her parents unexpectedly lost their jobs in Warsaw – her father at Warsaw School of Technology, her mother – at Warsaw University. It is quite possible that these events, so tragic for the family and the child, as she was at that time, evoked her empathy towards people around her. She tried to see people with their problems instead of indifferently passing by them. She helped as much as she could at the cost of her energy and time so precious. "I am going to the refugees' camp in Deheyshe outside Bethlehem to teach children English, are you coming with me?" She travelled there in her car, packed with pamphlets whenever she could. In 2004 she established and edited the Internet paper *Occupation Magazine* and became a volunteer helping a lot of people. She initiated the program for Palestinian schools in Al Khader. In her writings in

Occupation Magazine she depicted everything she saw around her; she also wrote in Nature a short text on Israeli-Palestinian scientific cooperation: "Israeli concern about Palestinian suffering", Nature 418, 479 (2002). She strived to help people; she saw a better future for the world by enhancing the understanding, the education and the development of all people.

Not in music or fine paintings
Not in great or courageous deeds
Not even in love -- shall wisdom lay;
Only in these things:
In earth in air, in pain and in silence.
(The Shell, A. Zagajewski, "Late Festival"; free translation from Polish)

It's been very difficult to believe that Victoria is gone. She left an unforgettable mark in each and every one of us, who were lucky enough to know her, a piece of her continually seeking and creative personality. -Joanna

ADVANCED SAMPLING METHODS

Prof. Michele Parrinello, Computational Science, Dept. of Chemistry and Applied Biosciences ETH Zürich, Lugano, Switzerland

Abstract: We introduce the well-tempered ensemble (WTE) which is the biased ensemble sampled by well-tempered metadynamics when the energy is used as collective variable. WTE can be designed so as to have approximately the same average energy as the canonical ensemble but much larger fluctuations. These two properties lead to an extremely fast exploration of phase space. An even greater efficiency is obtained when WTE is combined with parallel tempering. Unbiased Boltzmann averages are computed on the fly by a recently developed reweighting method [1]. We apply WTE and its parallel tempering variant to the 2D Ising model to Gō-model of HIV protease and the nucleation from the liquid state.

[1] M. Bonomi et al. J. Comput. Chem. 30, 1615 (2009).

SIMULATION OF REACTING FLOWS WITH STIFF SOURCES

Matania Ben-Artzi, Institute of Mathematics, The Hebrew University of Jerusalem, Israel

Abstract: The Z-N-D model serves as a basic model for compressible, non-isentropic flow subject to chemical transition, characterized as the transition from "unburnt" to "burnt" substance. It is governed by a "reaction law", relating the fraction of the burnt part to the thermodynamic quantities. The latter satisfy the compressible fluid equations (Euler equations), depending on the burnt fraction. The system is therefore coupled and becomes "stiff" as the reaction rate grows. The limiting case is that of an "infinitesimal transition layer", the so-called "Chapman-Jouguet (C-J) model". The subject of this talk is to describe the numerical simulation of the reacting flow and its ability to handle the passage from Z-N-D to C-J.

COMPETITIVE ADSORPTION OF HNO₃ AND HCL ON/IN WATER CLUSTERS AND ICE

Nevin URAS-Aytemiz, Dept. of Chemistry, Suleyman Demirel University, 32260 Isparta, Turkey

Abstract: The topic about solvation and ionization of strong acids such as HX (X=CI, Br) on/in hydrogen-bonded solid surfaces such as water and methanol ices have been subjected to many hot discussions and working times with Victoria Buch(1-3). There are lot of inspirations from those days in this work that deals with the competitive adsorption of two strong acids, namely, HCl and HNO3 on/in the water clusters and the surface of crystalline ice slab containing 72 water molecules produced by Victoria Buch at the average temperatures below 140 K. The main tool of this study is on-the-fly molecular dynamics as implemented in the density functional code QUICKSTEP(4)

which is part of CP2K package(5). The small water clusters containing both HNO3 and HCl with up to five water molecules were further checked with MP2 level ab initio calculations. The results will be discussed in terms of dynamics, structures, energetics and spectroscopic perspectives.

References:

- V. Buch, J. Sadlej, N. Aytemiz-Uras, J. P. Devlin, J. Phys. Chem. A (2002) 106, 9374.
- 2. J. P. Devlin, N. Uras, J. Sadlej, V. Buch, Nature 417 (2002) 269.
- 3. N. Uras-Aytemiz, J. Sadlej, J.P. Devlin, V. Buch, J. Phys. Chem. B 110 (2006) 21751
- 4. CP2K, http://cp2k.berlios.de (2000-2004).
- 5. VandeVondele, J.; Krack, M.; Mohamed, F.; Parrinello, M.; Chassaing, T.; Hutter, J. Comp. Phys. Comm. 2005, 167, 103.

This work was supported by TUBITAK (Project number: 107T044)

SOME PEOPLE BE-COME MILESTONES IN ONE'S LIFE

Victoria was one of the milestones in my life. Thanks that she was in my life! She was my role model as a scientist and human being. I had an opportunity to work



Paul, Victoria, Nevin and Udo (Poland, 2003).

with her as a postdoc and later as a collaborator. One of the good things that I always admire about her was how she could make the complex problems as simple as it can be.

She is still living in my daily life, since whatever I am doing, there is always something from her, i.e. her words, thoughts, programs etc. I have only one wish that I like to be like her as a scientist and human being... -Nevin

THE RAVEN-HAIRED WOMAN

Audrey Dell Hammerich, University of Illinois at Chicago

The projects on Taylor Street in Chicago, near the University of Illinois, are no more. One can debate whether that is progress or not. But fifteen to twenty years ago the young Afro-American children were full of smiles and laughter as a curly, raven-haired woman distributed quarters as she walked from her office in the Chemistry Department down Taylor Street to her favorite cafe to have a good cup of coffee.

Twenty-, thirty-, or perhaps it was a forty-block walk in a warm Chicago rain deep in an animated, free and easy conversation that knew no bounds: people, politics, secrets, and, of course, science. Much later the scene would switch to the Jerusalem Rose Garden and the much anticipated midnight walks with talk just as unfettered.

A cat would not fit in with the new life in Tel Aviv so out into the garden it goes. It cries, it is scared, it is miserable. It finds its place on the foot of the raven-haired woman's bed and remains her constant companion until the end.

The young teenage boys in the family are now probably too old to be driven (legally?) from their home in the West Bank, close to Jerusalem, to the sea where they would swim, laugh, show off their diving skills, watch over their younger sisters. But the raven-haired woman found the time to laugh with these children and provide them with a respite from the hot summer days and the isolation of their village.

These boys have a bright-eyed younger sister born with serious birth defects. The raven-haired woman became her advocate and arranged for and took her to her many operations which slowly, slowly began to transform her feet, hands, head, and face. They would both smile at each other and hold hands as they would leave the sea.

Buying a "new" carpet in the Old City was an adventure. So often Arabic prompts a Hebrew response. But not for the raven-haired woman. She had a naive determination to hold her own. She broke down the defenses, possibly with passable Arabic, but more her willingness to continue to converse and the engaging smile. It took a long time - no Arabic coffee necessary to create the mood - they were both engrossed in each other.

A partial list of favorite places: Prague, Lugano, Trieste, Telluride, Venice which were so generously shared. A passion for travel, knowledge, different cultures which could be entwined with people and the love for and pursuit of science. To work and play with gusto.

Superlatives abound - the generosity, the caring, the science, the magazine. So many lives have been enriched in so many different ways.-Audrey

STUDYING WITH VICTORIA

Noam Agmon, The Hebrew University of Jerusalem

I have told the following anecdote in the presence of Victoria, so I believe she would not mind me telling it in her absence, following her premature departure. In retrospect, I think this story teaches us something about Victoria's peculiar sense of humor and her devotion to scientific theory.

We have studied together for a Bachelor degree in chemistry at the Hebrew University, 1972-1975. During the first two years I did not know Victoria

well, as she was always busy with her studies. Then, in the third year we were paired-off for the advanced PChem lab. Our first experiment concerned gas-phase reaction kinetics. We have hardly begun the experiment, when Victoria broke a glass flask. First, she was dismayed. Then a naughty grin showed up at the corner of her mouth.

"Noam," she said, "as you can see I am not very good in experiment."

Then, she added: "You are probably not very good in theory (!). So let's make an agreement: You will perform the experiments, and I will do the computations".

At first I was surprised, then I agreed, and this is how we managed to finish the lab with distinction in spite of our mutual handicaps...

Years passed, Victoria and Ron returned from the US, and we were both faculty members in the same PChem department where we have conducted our first experiment. We both taught PChem to undergrads: Victoria always late, running to class with a pile of papers under her armpit.

Our daughter, Galit, found herself in the same class with Victoria's only daughter, Dassi, and they became good friends. When they reached highschool, they were paired-off for a biology experiment on osmosis. I wonder if it occurred to them that osmosis was part of the PChem syllabus that their parents were supposed to teach. And surely, they were not aware of how their parents were paired-off for a lab course a generation before. This time, however, both excelled in both experiment and theory. Thus, it is through our children that we get a second chance... -Noam

SAD NEWS...

Roi Baer, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, the Hebrew University of Jerusalem

Friends, I have sad news. A dear friend, teacher, colleague, and wonderful human being, Professor Victoria Buch, has passed away today, after a long struggle with a fatal disease.

I want to write a few personal words about the Victoria I will miss very much. Victoria the "real" person; very few are, in my view.

I see in Victoria a real scientist. She did not follow trendy puffs of wind; she chose instead to grapple with the more basic, deep and difficult scientific questions of chemistry. She had the "nose" for asking those really interesting fundamental questions in her field and the creativity to develop theoretical and computational methods to answer them. Some highlights of Victoria's career include the brilliant diffusion Monte Carlo method she developed for rigid bodies and her many important landmark works on the structure



Victoria in Morskie Oko, 1997

and spectroscopy of ice and water, their surfaces and their chemistry.

Victoria is a real human being. Yes, she was too often late to here and unintentionally absent from there... sometimes totally forgetting her schedule... or where she left her cell-phone... But I knew: this is just scratching the sur-

face. Actually, I always felt this "absent-minded-professor" was much more in touch with reality, connected to this world, than I will ever be!

This is because Victoria's eyes and heart were open to see and feel the harsh events around us here in Israel. She made no concessions, no compromise, always true to her conscious. She fiercely demanded and fought for justice and compassion in times few have the patience and integrity to rise above their anger to do so.

Victoria willingly paid a high price for her social and political activities. Few would be able to stay so scientifically prolific, highly cited and internationally acknowledged as Victoria while concurrently devoting a huge portion of their time and patience to actively help the weak, the vulnerable and the suffering.

Indeed, Victoria was constantly busy demonstrating, blockade-watching, writing letters, publishing petitions and lecturing about these "real world" matters! Some people in our department may have bitterly disagreed with her views and actions. But I am sure they were secretly impressed by her sincere and pure intentions realizing she was constantly searching for the 'good thing to do'. (And perhaps that made them even more cross...)

I was not a student of Victoria. Never took a formal course or class with her. But I learned a lot from her – just by watching. And she was a great teacher!

It is so sad for me that a beautiful person as Victoria was snatched from my world, so suddenly, so brutally and so much too early! - Roi Baer (Announcement to members and Beirat of the center)

OUR LAST ADVISOR

Barbara and Lukasz Cwiklik, Acad. Sci. Czech Rep.

We met Victoria in Prague, in winter 2007. She asked, "do you really have to go to the US? Don't you want to come to Israel?" and she invited us to do postdoc with her in Jerusalem.

We will always remember Victoria as a great advisor; not only regarding science. We remember our first day in Jerusalem. She visited the Old City with us and after two hours we knew exactly what we shall see and visit during the next two years. We visited both suk ans shuk, she said "if I could I would eat knafeh every other day!" and of course, in a few minutes we knew the best stands with cheese and pastry in the whole Israel. In the evening she took us to a fancy restaurant in East Jerusalem and gave us a list of other nice places to eat. Later, we found out that this list was precious and exact guide to the best restaurants.

There was that day, or rather evening, we remember very well. It was last June. There were four of us and we spent the whole evening at Victoria's place talking about science. She was so passionate despite the fact that from time to time one of us four was falling asleep, Victoria was not showing any signs of tiredness. During this talk we wrote down a few pages long plan regarding future research, a plan for us, not for her. That evening, talking about our decision where to go after staying in Israel, she said in her beautiful literary style Polish: "I am happy where I am, but if I were as young as you are, I would have made the same decision as you have".

She was our last advisor and we are proud to be her last students. – Barbara and Lukasz

LIKE IN THE MIDDLE OF THE CONVERSATION

Tova Feldman, The Hebrew University of Jerusalem

I just arrived back from Copenhagen, and read that Victoria left us. I knew It could happen any minute, and yet I was a little bit hoping for miracle.

BUT VICTORIA DID NOT WAIT FOR MIRACLE! She said it almost explicitly. Maybe this fact can console her beloved sister NINA and daughter Dasi. I mean the fact that she knew that she is facing the end, and with all her pains and understandings behaved as a QUEEN, she succeeded to organize life after life.

I saw her about two weeks ago, when she invited some friends for Audrey's birthday...She thought of everything. To finish as much works as possible, to find the persons with whom her students and colleagues would continue their research instead of herself, to suggest the last book she loved, and I am sure in many other issues she looked for someone instead of herself....

Victoria dear, so many subjects were on schedule between us, and you left just like that in the middle of the conversation. - Tova

VICKYNESS

Mark Ratner, Northwestern University

Victoria Buch was a scientist in the deepest sense. She cared about truth, and about understanding, and about other scientists. She understood how demanding science could be, and was willing to play the game at the very highest level. She understood that our tools are necessarily blunt instruments, and that we can only quarry real insight with them by trying to improve their sharpness, and by working with them all the time, very hard, before anything significant happens. But she also understood that the game, though hard, is wonderful – that understanding the world, and predicting its

behavior, is an opportunity that has only been afforded to us very recently in the history of man, and even more recently in the history of the Jewish people.

When I first came to Jerusalem, invited by Rafi as part of the Advanced Study Institute, I met this remarkable woman from Poland, who was a gusher of enthusiasm for science, for scientists, and for theory. I remember staying up very late trying to understand why our self-consistent vibrational equations didn't converge. I remember haggling with Vicky over pitas at an outdoor grill, trying to express the error terms that arose in the vibrational analogs to the Hartree-Fock equations in a way that looked a lot like MP2 theory. And I remember scheming with Victoria about different semiclassical approaches, different ways to improve the solutions.

Since that time, Victoria and I went in very different directions with our science. But whenever I saw her at a meeting, the same intensity, the same creativity, the same unique Vickyness were always there. She got interested in water, and ice, and Car-Parrinello calculations, and the mysteries that occur at the interface of ices. But she still had that remarkable flair, the openness, the curiosity, the delight when things happened right.

I firmly believe that the graduate students in Jerusalem are the best that I have ever encountered. Victoria was the first of them whom I really knew well, and she set an extraordinarily high standard for this, as for almost everything else that she did.

Her loss leaves a huge hole. There's a hole in the faculty of the Hebrew University, there's a hole in the community of theoretical chemistry, and there is a hole in my appreciation of the science that we all do. I have learned a lot from many people at the Hebrew University, and working with the theoretical chemists there has been one of the great joys of my career. But Victoria was perhaps the most free-spirited of all of us, because her enjoyment of science seemed to be entirely dissociated from some of the shabbier considerations, like getting funded, and the size of an office, and credit.

It was a privilege to work with Victoria, from her time as a graduate student through her time as a Full Professor. If there were more people like Victoria, theoretical chemistry would be a better place. We were all privileged to know her, and to work with her, and to learn from her.

May her memory be for a blessing. – Mark Ratner

VICTORIA BUCH. MEMORIES OF CLARENCE AND JOAN MUSGRAVE, ST ANDREW'S CHURCH JERUSALEM, 2000 - 2006

Mattanjah de Vries, University of California, Santa Barbara

Ours was an unlikely friendship, which started in an unusual way.

My wife and I had arrived in Jerusalem in July 2000, to work at the Scottish Church, when there was that mixture of optimism and apprehension. Camp David came and went, the Intifada started, and was in reality to be with us until we returned to Scotland in 2006. I am a Church of Scotland Minister, having worked for a short time in the USA, a longer time in Zambia, and an even longer time in Edinburgh.

Quite early in the Intifada, Victoria wanted to get some assistance to a friend in Hebron – not the easiest of things for her to arrange. In contact with a professional colleague and friend in Prague, he suggested that she get in touch with the Church of Scotland Minister at St Andrew's Scottish Church in Jerusalem, whom he knew. Victoria did that, introducing herself at the very outset as a "third-generation atheist." Labels being unimportant on this occasion, I was able to arrange for her assistance to reach her friend in Hebron.

From this unusual starting point, our friendship developed. We learned a great deal from her – of her background, of her family, of her commitment

to opposing the policies of successive Governments of Israel, and of her seemingly boundless energy.

Letters used to find their way from my wife and myself to friends in different parts of the world, telling of our experiences, and sharing the stories of folk such as Victoria. Without ever asking for donations, money did arrive to be used as the need arose.

Victoria had a good sense for the scent of money, and the people who had donated it were more than happy to have her use some of it. Early in our friendship, we were standing one day at the Women in Black demonstration in Jerusalem. Our conversation was short and to the point. "I need money", said Victoria. "What for?" said I. "Expenses for an operation for a girl from the West Bank," said Victoria. "How much?" said I. "\$5,000.00," said Victoria. "Done," said I. The money was available, the operation was carried out, and we became friends with her friends.

It was a recurrent theme of our friendship – the third-generation Jewish atheist asking the Scottish Presbyterian Minister for money to help her Arab Muslim friends – or to help with some of her other commitments. It was a demonstration of what can be done, and an illustration of what should be done by people of different backgrounds, and one which we valued enormously.

Victoria was convinced that we needed "to be educated," and we were more than happy to accept her as our teacher. We met her family, some of her friends, and accompanied her on expeditions to different parts of Israel, and even on one occasion to Hebron. She was a good teacher, and our lives have been enormously enriched by having known her.

In 2008 she was able to stay with us in Edinburgh, and we in turn stayed with her in Jerusalem. Sadly, such visits are now things of the past. I am not quite sure what her final greeting would be to us – but it would be entirely

in keeping with the sort of friendship we had were she to be asking if we had any money for one of her Arab friends. Assuming that third-generation atheists get to heaven, I would not be surprised to learn that she is busy organising folk there, encouraging them to log-on to www.kibbush.co.il.

Our lives are richer for having been able to share them with her, and they are now poorer for her passing.

Victoria was my neighbor in the Institute of Chemistry: her office was next to mine. At times she would brew coffee; we would free up a chair by pushing aside piles of papers and talk — some science but mostly politics. Her sharp, incisive analyses were delivered with a mischievous twinkle in her eyes. She taught me so much about life in the Institute, in Israel, and in the Middle East. Whatever the topic, Victoria dispensed her wisdom with a mixture of humor, true caring, and integrity. For all of these she will be dearly remembered and sorely missed. - Mattaniah

FOR HER SPIRIT AND IDEALISTIC PRINCIPLES

Michael Michman, The Hebrew University of Jerusalem

I was very sad and dismayed to learn of Victoria's passing away.

Our research activities were far apart but I had outstanding opportunities of acquaintance with her during my tenure as head of school in the nineties. She then took upon herself one of the most difficult undergraduate courses on The Chemical Bond, which was often too difficult an obstacle for many of the students. She expected others to rise to her level. She ran the course with great dedication, enthusiasm and uncompromising approach as befitted her personality while I found myself a proponent of a different didactic approach proposed at the time as an alternative, even if that would get the students only halfway - though safely, through the subject.

Our tasks were different. We had great fights and she did not spare me, but I respected her deeply, even envied her, for her spirit and idealistic principles. I do not think it was mutual. In our research and particularly in our teaching assignment we may strive for the maximum and sadly, often settle for the possible. But it is pathfinders like her that we really need.

She will be badly missed. - Michael

WHAT GRANDMA WOULD THINK ABOUT SUCH TALK

Dor Ben-Amotz, Perdue University

I was fortunate to have encountered Victoria while I was on sabbatical at the Hebrew University in 1994. I soon came to realize that she was a member of that rare sub-species of great scientists who are fascinated equally by the idiosyncrasies of people and the molecules out of which they are composed.

One of my early conversations with Victoria took place when she found me sitting on the grass drinking coffee near an outdoor kiosk at the Hebrew University. Conversations with Victoria often took interesting turns, and this one drifted into existential territory about why we do what we do. Victoria was clearly amused by the naivety of my evident misconception that such topics had anything to do with reality. Her perspective became most apparent when she wondered what her grandmother would have thought about such talk.

Before long Victoria and I were making plans to get together with Stephanie (my wife) and Dassi (her daughter), as well as Nina (her sister) and other friends and relations, for various adventures. These included visits to exotic tea houses and restaurants in the back streets of Jerusalem (both east and west), as well as hikes and picnics in the Jerusalem hills. Our encounters later extended to more far flung locations, from star gazing in Ein Hod to

kite flying in the Berkeley Marina, and a surprising encounter between Victoria, Nina and my mother while waiting for the Gordon conference bus to New Hampshire.

Victoria and my mother grew independently fond of each other, which I was very pleased to see. I also have Victoria to thank for introducing me to other fine specimens of our species, including Pavel Jungwirth and his family, who later led Stephanie and I on a memorable adventure in the Sumava mountains south of Prague. I have learned to expect that any friend of Victoria's is sure to be someone I would be fortunate to get to know.

Although Victoria's political views and courageous actions may have been perceived by some people as arising from the ideological far left wing of the Israeli political spectrum, Victoria was actually not the least bit ideological. Rather, her political views were motivated entirely by common sense and human compassion. When she perceived injustice, hypocrisy, or idiocy she never hesitated to point it out, loudly and clearly, in person or to the wide world, as she did weekly in her widely circulated compilation of news clippings and stories from around the Middle East.

Victoria has broadened my perspective and set me straight regarding what is really most significant and valuable. I still have much left to learn and will sadly now have to make my own fumbling way without her expert guidance and fine fellowship.

DEDICATED AND HUMANE PRESENCE

Stephanie Ben-Amotz, Perdue

I am neither a colleague nor a close friend. I like to think that had we been within 100 mile radius of each other more than a few times in our lives, we would have developed a stronger friendship. But I want very much to write about her. I met Victoria in Jerusalem in 1995. My husband was on a sabbat-

ical at the Hebrew University. Soon after arriving, Dor came home talking about someone named Vicki who, he informed me, was great and I would like her. My first meeting was actually over the phone, and odd as that may sound, I adored her immediately. We had chatted in passing a few times, and were planning to all go hiking together. I made some little comment about finally getting to "see her in the flesh" which for some reason she found the idea of looking forward to THAT very amusing, and she started to laugh and sputter a bit, and tell me in a booming voice that she was not much to see, which of course was not true. She was much to see.

I feel the loss of her is twofold, an unfathomable one for those who cared about her, but also the world has lost a very dedicated and humane presence. I saw her as a person of rare conviction. She was courageous and honorable and kind. I liked and admired how she conducted herself in the world, if that makes any sense. I loved being around her and Dassie, the two of them were funny and sweet together and challenged each other a lot. I have a great memory of sitting on a rooftop with them in Ain Hod, looking at the night sky and talking and laughing in the dark.

It is very sad to no longer have her here on earth. -Stephanie

WE MET AT A CONFERENCE ON WATER

George Reiter, Dept. of Physics, University of Houston, and a producer of the radio show Thresholds, on KPFT in Houston

Her work was central to the field, and creating a stir. I was impressed with her relationship to her work, concerned only with the substance of it, quite as willing to give credit to others as to call them to account for their oversights or challenge them on their mistakes. We found we shared a commitment to justice, fair treatment for all of humanity, and as Jews inheriting a tradition of acting in the face of injustice, a need to act on the expropriation of the Palestinians, the occupation of their remaining land and their continu-

ing mistreatment by the Israeli state. She did this in many ways, as I came to find out. One of which was her nearly weekly posting of "Today's Headlines in the Occupation Magazine", posted until two weeks before her death, to which I became a subscriber. She had contacts with the resistance to Israeli government policies in Israel and Palestine. She used those contacts to bring the voices of the resistance in its many forms to the United States, where the Women in Black, the Combatants for Peace, the Anarchists Against the Wall , Rabbi's for Peace and others were given time on my weekly radio show to share who they were and what they were about to an audience who rarely heard about them, and for the most part, didn't know they existed. It is difficult to hold out with intelligence and integrity a path to the future that is disavowed and attacked by those in positions of power in your own country, particularly when the mantra of survival as a nation is trumpeted at every turn, and used to excuse every barbarism. Victoria did just that. Her bravery, intelligence and wit will be missed. Her support for the struggle to free humanity from the ghosts of the past will have consequences for all time.

EMAILS EULOGIZING VICTORIA

DEAR ROI,

Sad news. When I think of Victoria I can clearly see her face and hear her rolling laughter, I think of her when she is talking with such enthusiasm and with such love on her science. She was a very warm person who worked on the physical properties of ice and really wished to make our world and our country a better place to live in. I am sharing with you and with all the members of Fritz Haber, the sorrow for the loss of a friend and colleague. Please give my condolence to her daughter and to her family. - Nimrod Moiseyev, Technion, Haifa

DEAR DASSI,

We don't know each other but now that you send also to me this letter, I want to express to you how much your mother is in my thoughts these days. Though never having been very close, we cooperated through the years on getting things published in the field of peace activism and I also became one of the editors of Occupation Magazine which she founded. Rereading her January article, now republished on Occupation Magazine, I feel she wrote it knowing that this was the end of her life, and maybe her last opportunity to add her very argued and penetrating voice. I hope that after the shock passes you will be able to live your life without her keeping a fond memory of her. Your mother, she was not just somebody.

Yours, - Beate Zilversmidt

DEAR DASSI,

I never had the opportunity to personally meet your Mom but, I knew her through her illness. I too have Stage III C Ovarian Cancer and have been struggling with this beast for almost three years. Viki and I shared our experiences with chemo that ravages the body but, not the souls of strong women. I read her articles and so did my GYN/Oncologist at the Seattle Cancer Care Alliance. His family lives in the West Bank and he so appreciated her zeal and brilliance as an accomplished scientist as well as pacifist.

She related her care in Israel at the University and how important life was and that she would try anything that could possibly give her better quality of life. I suggested that she come to Seattle for an opinion and that we had a bedroom just for her if she chooses to do so. She had been here before as I recall and had friends at Puget Sound U.

Once I asked what she did in her work life. When she mentioned she dabbled in "quantum physics" I was impressed for sure and didn't make further inquiry since my knowledge of that particular part of the universe is limited to say the least.

I have tried to reach her in the last couple of months and was concerned that I hadn't heard from her. My condolences are with you and her family and friends and I am so saddened to her of her loss.

I pray for peace in the world. - Cathi Anderson

DEAR DASSY,

My deepest sympathies to you all on the death of your mother - this is my tribute to her - she meant a great deal to me. Victoria was one of the most courageous women I have ever had the privilege to meet. Her unflagging work to expose and to try and alleviate the terrible injustice under which the Palestinians have to live was an inspiration to me and to many fellow Scots who also knew her. She never faltered in her task although her academic career must have been threatened nor did she falter when she became ill. I saw her in Edinburgh last year and her energy seemed undiminished. I thank God that there are Israelis like her and I hope and pray that those of us who believe as she did in justice and then peace will continue the struggle however longs it takes.

Dr. Runa Mackay - I lived and worked in Israel and with the Palestinians from 1955 until I retired to Scotland in 1995.

DEAR DASSY,

It's for me such a sad task to write appropriate words as a dedication to Victoria's memory. When I knew her several years ago in Jerusalem during a vigil of "Women in Black" I was much impressed by her strong engagement for a just peace. Later she came even to Germany to inform people here about the efforts of Human Rights groups to fight for the end of the occupation and a just solution of the conflict. When I had invited her to our "Middle East Peace-Group" she didn't hesitate to come to us and tell us about her experiences as a Machsomwatch woman. Her lively report about the humiliating measures of the soldiers towards the Palestinians was such an important message and unique for most of our members. She also joined us with another Machsomwatch woman who also visited us reporting about her work near the checkpoints in the Occupied Territories. Last not least I want to appreciate her weekly choosing headlines for the Occupation Magazine and sending it to many people. It is so important to receive such alternative messages! It is so painful to miss her vivid, strong personality. She was a

wonderful woman and I will never forget her!

Annelise Butterweck, Bergisch Gladbach

QUEEN VICTORIA

Victoria seemed to me to be a force of nature. She was a leader in her scientific field and always seemed to be working on the hottest and most important problems with others desperately trying to catch up. Then there was her commitment to the peace process in Israel and her bravery in fighting for the human rights of Palestinians when the easiest thing to do would have been to have kept quiet. I first met her when I was but a lowly graduate student and even though I was not and never will be in her intellectual league, she always made time to talk, gossip, tell jokes and offer advicewhich I rarely took, though should have. She was a friend to many young scientists and we genuinely enjoyed her company. No, I didn't know her that well, but I always secretly idolized her for her brilliance and her humanity. I once called her 'Queen Victoria' because to me, she was royalty- a towering presence and an icon, but also someone who looked out for us like a favorite aunt.

Christian Burnham, University of Houston

HI TOVA,

I have just known from Christiane (she knew from you) that Victoria passed away. It's a very sad new. Victoria was always very warm with we all "visitors", and one of the responsible people for us losing very fast that label ("visitors") to feel as one more in F.H.

I won't forget helping her doing some phone calls to a lost village of Central America when she was organizing one of her crazy holidays. She was a good scientific, but also a very amusing person.

All my condolences to all of you, their colleagues and friends, in F.H.

hugs.

Jose Palao, University de La Laguna, Spain

GENEROUS, DEDICATED AND CARING INDIVIDUAL

I was very sad to hear about her illness, then shocked by her death. We first met in Jerusalem in 2004, having been in email communication for some time – she always made herself available via email and in person. Her contribution to informing the world about Israel/Palestine by founding Occupation Magazine was invaluable. She will be sorely missed. My condolences to her family, friends and colleagues.

Vivien Lichtenstein, Jews for Justice for Palestinians, UK

VICTORIA

I sent this message via Adam Keller on 24 June as soon as we heard from him of Victoria's death: I'm stunned to learn of Victoria's death. We so admired the energy she put into her work and the Occupation Magazine website. Please pass on my personal condolences, and those of Jews for Justice for Palestinians, to her family and friends and to all who work on the Kibush project.

Richard Kuper, Jews for Justice for Palestinians, Information Officer

COURAGEOUS PERSON

I met Victoria in the early 1980's at the Fritz Haber Institute, when I was a Master's degree student and Victoria was finishing her PhD with Bennie Gerber as her dissertation advisor. Victoria was one of the most exceptional persons I knew. She was a truly passionate person, with an open heart and broad-minded intellectual spirit. While her chief commitment and passion was science, she was also deeply read and interested in literature, philosophy, music, politics, art, and more. One could see her delving into Paul Dirac's Principles of Quantum Mechanics, her favorite textbook, but she was also reading and discussing Descartes' Principles of Philosophy. Victoria read and loved Dostoyevsky, Camus and myriad other writers. While Victoria's mind was attuned to the fundamental and the abstract, she also was interested in and understood the-down-to-earth and the practical. Perhaps this was one reason she was such an excellent teacher: she knew and loved the

theories and foundations, but at the same time she understood the mundane frame of mind and limitations of her students. I was not in contact with Victoria in later years, when her career as a theoretical chemist flourished, and at the time she was also devoting much of her time and energy acting for peace and justice in the Middle East and helping the disadvantaged and helpless. I only learned about this chapter in her life during a recent visit to Israel, after her passing. But I was not really surprised to learn of her activities during the past several years. Victoria was a very courageous person who fought for her convictions and she was a very generous and in many ways a selfless person. She certainly was a very exceptional individual. I will miss her. - Michael Chayut

DEAR BENNY,

I just learned today that Victoria Buch passed away in June. What sad and terrible news. I spent a week with Victoria last summer in Telluride. I had heard that she was ill, but her trademark vitality and wit were present in full force, and she never let on. I will miss her deeply. She was a proud member of the Fritz Haber Center and a wonderful diplomat for chemistry. There are so few like her.

I also learned today from an internet search about her activities on the part of Occupation Magazine. I did not know about this side of her; she was even more remarkable than I knew.

I hope that all is well with you, and I look forward to seeing you sometime in the future. Gil Nathanson, August, 6 2009, Dept. of Chemistry, Univ. of Wisconsin-Madison

IN MEMORIAM

Victoria Buch, Hebrew University Professor, TSRC Organizer

TSRC lost a long-time friend and supporter, and the world lost a brilliant scientist and compassionate humanitarian, when Victoria Buch passed away on June 21, 2009. Over the last decade, Viki frequently made the long journey from Jerusalem to Telluride to participate in TSRC workshops, and during the last eight years she organized a biennial workshop on the properties

of liquid and solid aqueous interfaces, which regularly attracted one of TSRC's largest contingent of scientists from around the globe. Viki was respected and loved by her colleagues who appreciated the rigor and creativity of her research, and cherished her contributions to the spirited discussions that are the hallmark of TSRC workshops. Although not well known to all her scientific colleagues, in addition to being an exceptionally creative, hardworking, and successful scientist by any measure, Viki tirelessly dedicated herself to the advancement of the rights and wellbeing of the Palestinians in the Occupied Territories.

Most of us would be content to make meaningful and lasting contributions in one arena. Viki showed us that it is possible to do much more. She will be sorely missed by all who had the good fortune to know her.

- Doug Tobias, UC Irvine, TSRC Board Member