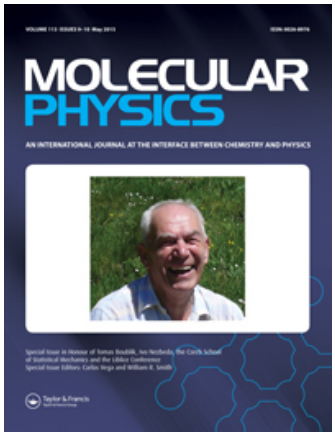

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Reminiscences about Tomáš Boublík, Ivo Nezbeda and the Liblice Meetings on the Statistical Mechanics of Liquids

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FOREWORD

Reminiscences about Tomáš Boublík, Ivo Nezbeda and the Liblice Meetings on the Statistical Mechanics of Liquids

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1. Tomáš Boublík, 6 May 1934–8 January 2013

It is our (William (Bill) Smith and Carlos Vega) great pleasure to offer the following introductory remarks for this Special Issue of Molecular Physics in celebration of the scientific contributions of Tomáš Boublík, the 70th birthday of Ivo Nezbeda and the contribution to the furthering of scientific research by the Liblice Conferences on the Statistical Mechanics of Liquids.

Tomáš was born in Krivoklat, Central Bohemia. After completing his high-school education in Rakovnik, he entered the Prague Institute of Chemical Technology and received his Diploma in 1957 for experimental work in the field of inorganic technology, and his Ph.D. in physical chemistry from the same institution. According to the regulations of the Communist regime of the time, he was required to spend a minimum of a year in 'working class employment', and he spent the time in the laboratory of the Research Institute of Inorganic Synthesis in Pardubice, a branch of a large chemical company. At the end of the year, Professor Eduard Hála, a famous Czech thermodynamicist, brought him back to Prague to join his group in the Institute of Physical Chemistry of the Academy, which then moved to the newly founded Institute of Chemical Process Fundamentals (ICPF) of the Academy, where he worked until 1992. In 1967–1968, Tomáš spent a year in Canada as postdoctoral fellow working with Professor G.C. Benson in the National Research Centre in Ottawa. In 1977, he defended his D.Sc. thesis entitled 'Statistical-thermodynamic study of liquids and liquid mixtures'. In 1989, he was a visiting professor at the Universidad Complutense in Madrid, Spain, where he first met Carlos.

During the Communist era, there was a sharp separation between universities and the institutes of the Academy (the equivalent of 'National Research Laboratories'). With only a few exceptions, people from the Academy were not allowed to teach at universities. Thus, only after the 'Velvet Revolution' he was allowed to defend his Habilitation thesis, which he completed in 1990, entitled 'Perturbation methods used to determine the equilibrium behaviour of liquids', to become an associate professor at the Prague Institute of Chemical Technology. In 1992, he left the academy to become a full professor in the Department of Physical and Macromolecular Chemistry at Charles University, where he worked until his forced retirement in 2005. Tomáš immediately joined the Chemistry Department at J.E. Purkinje University in Ústí nad Labem, at the invitation of Ivo Nezbeda. Many researchers complain about teaching duties but never Tomáš. He really liked young people and tried to make a positive impact on the younger generation.

Although Tomáš started his scientific career as an experimentalist, he was convinced by Professor Hála to turn to the molecular view of matter. After some hesitation, he took up this view seriously with his first Ph.D. students, Karel Prochazka and Ivo Nezbeda. He established his reputation by his studies of fluids composed of hard-body objects of various shapes, and remained faithful to this topic for his entire career. He was the first to publish [1] what has become known as the Boublík–Mansoori–Carnahan–Starling–Leland (BMCSL) equation of state (EOS) for hard-sphere mixtures, and another equation referred to by his name is the Boublík–Nezbeda equation for hard dumbbell fluids [2]. The seminal paper by Tomáš and Ivo [3], '*PVT* behaviour of hard body fluids. Theory and experiment' became the bible for the field, and although it was published in the somewhat obscure *Collection of Czechoslovak Chemical Communications*, it has over 325 citations. In addition to his 151 original papers (more than half of them single-authored), he also published, with Ivo and K. Hlavaty as co–authors, a monograph on the statistical thermodynamics of simple liquids and their mixtures [4].

Some of Tomáš's colleagues say he was somewhat of a pessimist and hard to get to know, but once you crossed

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this small barrier, you realised he was one of the most friendly and kind persons you would ever meet. An amusing example of his pessimistic nature that caused him some grief occurred when he visited Canada in 1967–1968, after several previous failed attempts under the Communist regime to obtain permission to allow him to leave the country. Having heard stories about the extremely cold weather in Canada, among other things, Tomáš decided to bring along a very heavy coat, and fearing it would be very cold on his arrival (even in the summer!) he decided to wear it when he exited the airplane in Ottawa. He thereby stood out markedly from everyone else, and looked so strange to the customs and immigration officials that they pulled him out of the line and sent him for a special examination to check if he had some type of communicable disease.

A nicer story concerning Tomáš occurred many years ago at ICPC, as recounted by Ivan Wichterle. Wichterle had supervised the Diploma thesis of a female chemistry student, and after the thesis defence a small celebratory party took place in the Institute. Tomáš was a bit 'under the weather' (but still 'in control'), and his male colleagues insisted that he accompany the student to her home in Sedlec, a small village just down the hill from the Institute. Thus, began Tomáš's courtship of his wife-to-be, with whom he ultimately had two lovely daughters and to whom he was happily married for the rest of his life.

Tomáš collaborated with several scientists, but probably the longest collaboration was with Ivo Nezbeda, who completed his PhD under Tomáš's direction in 1974. It was a rather interesting symbiosis between their two different characters. Their close relationship, both scientific and personal, lasted until Tomáš's death. Approximately at the same time when Tomáš was forced to retire and leave Charles University, Ivo became Chair of the Chemistry Department at the newly founded Faculty of Science at J.E. Purkinje University in Ústí. In order to strengthen the research capacity of the department, Tomáš was his first choice. He immediately accepted the invitation without any hesitation and started regularly commuting to Ústí, about 100 km away from Prague. He really loved students and teaching.

Bill first met Tomáš in July 1978, when he spent three weeks at the ICPF under a Canada–Czechoslovakia exchange program, during which time a paper was completed by Bill, Ivo and Tomáš from start-to-finish [5]. Carlos met Tomáš for the first time at the IUPAC conference in Lisbon in July 1986, when he was a final year–student of chemistry at U. Complutense in Madrid. His undergraduate thesis dealt with perturbation theories of liquids using the Kihara potential, so he had read many of Tomáš's papers. He was nervous when invited to dinner with Tomáš, along with Prof. Lago and Diaz Peña from his Department. Carlos still remembers the excitement he felt at the prospect of not only being at his first international conference, but also of sharing a table with one of the scientists whose research was so well known to him. He found Tomáš to be not only an excellent scientist, but also a very nice person (the experience of both Bill and Carlos indicates that the two aspects are not always simultaneously observed in a given person).

In the autumn of 1989, Tomáš visited Madrid for a sabbatical leave organised by Prof. Diaz Peña, one consequence of which was a joint paper with Peña and Carlos on the EOS for mixtures of chain molecules [6]. By that time Carlos was a Ph.D. student, working under the supervision of Prof. Lago. Tomáš was in the Department from September 1989 to July 1990, and during that time, Carlos had the opportunity to get to know Tomáš much better. On the professional front, they became involved in two research projects, both of which led to publications [6,7]. Carlos notes: 'I have been very fortunate to work with a number of very good scientists that have deeply influenced my view of science. Tomáš is certainly one of them. Every day we discussed the progress of the research. My duty was to perform computer simulations of mixtures of hard-sphere chains. Even though I made several mistakes, which somewhat delayed the research, he was always patient with me, pointing out the origin of my mistakes, and emphasizing that you learn much more from your mistakes than from anything else. The image of working with Tomáš is always present in my mind whenever I now do research with my students and things do not work out as planned'.

Carlos recalls: 'Tomáš used to come to lunch with several colleagues from the Department. After lunch it was coffee time and a traditional Spanish game played with some coins determined who was to pay for the round of coffee. Many scientists from all over the world have been tested in Madrid by means of this traditional game, and the results are often surprising! During his sabbatical stay, Carlos and Tomáš got along very well, and together visited places such as Toledo, Segovia and the mountains close to Madrid. They had the opportunity to talk about many things. Spain and Czechoslovakia were certainly very different countries, but they both share some things: a war (a civil war in the case of Spain), and the Second World War in the case of Czechoslovakia. These wars changed everything for the people of both countries. Tomáš was the same age as my father, and I realised then how, in both cases, to be born in 1934 was an initial condition that would determine much of the rest of your life'.

But life changes from one day to another, and that was the case in the autumn of 1989, when the world changed in a few months. After the fall of the Berlin wall, the Velvet Revolution changed the landscape of the former Czechoslovakia in just a few months. Tomáš complained that he had been waiting for a moment like this for more than 55 years, and the change happened just at the time he was on sabbatical leave in Madrid. He was very enthusiastic about the coming new era. It is probably true though that sometimes reality does not correspond with the image one has

in one's dreams. After returning from Spain, Tomáš joined the Charles University.

On 8 January 1970, Tomáš submitted to the *Journal of Chemical Physics* a two-page paper containing a new EOS for hard-sphere mixtures, an extension of the famous Carnahan–Starling EOS for pure hard spheres [8]. At that time, submitting a paper to the *Journal of Chemical Physics* written by a single author from Czechoslovakia was not as usual as it may appear (as is easy to check using the Web of Knowledge). Submitting good papers to good journals certainly increases the visibility of one's country in the international community. The paper was accepted and published [1], along with a comment by Carnahan and Starling [8]. In 1971, Mansoori *et al.* [9] published the same hard-sphere mixture EOS, which has come to be called the BMCSL EOS. Carlos observes: 'Reading the three papers [1,8,9] is, in retrospect, an interesting exercise. I have been to conferences where some well-intentioned (but perhaps somewhat lacking in historical perspective) young people mentioned the "Mansoori *et al.* EOS for hard sphere mixtures", when Tomáš was also in the audience'. Tomáš usually never raised his hand to point out that this equation had actually been published by himself for the first time on 15 July 1970. Tomáš was very modest that way. However, his friends, collaborators and colleagues recognise his many contributions to science, his will to put his country on the scientific map, and his quiet effort to develop a better future for new generations of young scientists.

Tomáš made significant contributions in the field of perturbation theories and in the development of equations of state of hard convex (and non-convex) fluids. His 151 publications have received about 3600 citations thus far. No doubt, he is one of the most highly cited scientists of the Czech Republic of his generation that started their careers in the early fifties. His papers on the EOS of hard-body systems will be very useful well into the future [1,10–14]. Carlos remembers: 'It was a pleasure and an honour to know Tomáš, and for me he was always an example to follow. Thank you for all, Tomáš'.

2. Ivo Nezbeda, born 20 November 1944

Ivo was born on 20 November 1944 in the small town of Chocen, 140 km east of Prague in eastern Bohemia. His father was a school teacher (of mathematics and art) and was also deeply involved in Czechoslovak soccer, ranging from being a first-division referee in 1946–1948 to coaching the Czechoslovak national soccer team in 1954–1958. This explains Ivo's avid interest in sports. He played on the top Czechoslovak soccer junior team, Sparta Prague, in addition to playing tennis and ice hockey; he continues to be an active tennis player and downhill skier even today. Ivo's father was also an excellent chess player, as was Ivo himself, who competed as a junior at the national level. Nonetheless, we recall Ivo telling the story that his father regularly won chess matches against him well into his 80's. Both Ivo's parents lived to a ripe old age, and hopefully their longevity genes have been passed on to him.

Ivo received his Diploma from Charles University in 1968. He originally had dreams of becoming a nuclear scientist, but this avenue was not possible, so (luckily for his future colleagues) he studied theoretical physics instead. He received his RNDr. at Charles in 1972, based on his original (alternative) analytical solution of the Percus–Yevick integral equation for hard spheres [15], followed by the solution for sticky hard spheres [16], and his Ph.D. in physical chemistry in 1974 at the Academy of Sciences in Prague at the ICPF under the supervision of Tomáš Boublík. He received his D.Sc. in 1989 in chemical physics, also from the Academy of Sciences. After the Velvet Revolution, he began teaching at his alma mater, in the Faculty of Mathematics and Physics, and was awarded a prestigious professorship in theoretical physics from Charles University in 2001.

Ivo's first employment was at the ICPF in 1974, which was headed at the time by Eduard Hála, a famous Czech thermodynamicist. Ivo worked in the group of Professor Boublík, and he still holds a part-time appointment at the institute. He rose through the ranks, becoming a Distinguished Research Scientist in 1989. He began collaborating with the Physics Department at J.E. Purkinje University in 1997; he joined the university as a Professor of Physics in 2005, and has been the Chair of chemistry since 2005. He also concurrently chaired the Department of Informatics at Purkinje for two years, and during the period 2006–2009 he was the first Chair of the Academic Senate for the newly established Faculty of Science.

In 2009–2011, he chaired the evaluation panel in chemical physics and physical chemistry of the Czech National Science Foundation (the Grant Agency of the Czech Republic), and in 2014 he was appointed Chair of the Expert Panel in chemistry serving the Government of the Czech Republic to evaluate research institutions nationwide.

Bill first met Ivo in the summer of 1977 at the Gordon Conference on Liquids, during the time when Ivo was beginning a postdoctoral half-year with Tom Leland at Rice University in Houston, Texas. Bill was then spending a sabbatical leave with Doug Henderson and John Barker, famous pioneers of modern molecular theories of liquids, at the IBM Research Laboratory in San Jose, California, and Ivo took the opportunity that fall to visit all three colleagues in San Jose. During that visit, he spent a weekend with Bill and one of his IBM colleagues and their families at a rented cottage in Lake Tahoe. While all the other adults took the opportunity to investigate the casinos in nearby Reno, Nevada, Ivo and Bill remained to babysit the five children. They consumed several bottles of beer in the course of a great scientific discussion, laying the groundwork for Bill's first visit to Ivo in Prague in 1978 and for their life-long collaboration and friendship. Since that time, Ivo and Bill

have been close friends and scientific collaborators, and are co-authors of more than 40 journal papers up to the present time.

Ivo has always been interested in both theoretical research and molecular-level simulation techniques in the statistical mechanics of fluids; he prefers to avoid the beaten path, but rather to develop new approaches and ideas. With a strong physics background and being surrounded in his workplace by chemists and chemical engineers, he has come to understand the importance of basic research for applications, and the primary application domain of his research has thus been fluids of chemical engineering interest.

Ivo made his initial professional mark in the late 1970s and 1980s by pioneering work, both theoretical and computational, with Tomáš on fluids composed of hard-body objects of different shapes. These activities began what has been referred to as 'the Prague School of Statistical Mechanics', and some of the papers have become citation classics [2,3]. The analytic equations of state that he and Boublík developed for hard-body fluids (e.g., the Boublík–Nezbeda EOS for hard dumbbells [2]) established his reputation.

In the 1980s, Ivo developed, along with Bill, the Reference Average Mayer-function (RAM) perturbation theory [17,18], perhaps the best available and most versatile perturbation theory for molecular non-associating fluids [19–21]. In the mid-1980's, Ivo and Bill developed a simple model of associating fluids [22] referred to as the 'Smith–Nezbeda" model' in one of M. Wertheim's early papers. Ivo and Jiri Kolafa later extended the model to a more elaborate version [23] which, in combination with Wertheim's thermodynamic perturbation theory, forms a basis for the very successful Statistical Associating Fluid Theory (SAFT), subsequently developed by Keith Gubbins and his collaborators, and now routinely used by chemical engineers for various applications and as a component of chemical process simulation software packages. Ivo continued to develop and apply theoretical results to chemical engineering problems, and in 1994 he developed, along with Jiri Kolafa, a non-empirical, molecular-based EOS for Lennard-Jones fluids, the most accurate equation for this class of fluids available to date [24]. He did significant research with Jiri and Bill on a general mathematical formulation of the global phase behaviour of binary fluid mixtures in the late 1990's [25,26].

Ivo began to concentrate on computer simulation methodology beginning in the late 1980's, and continues this emphasis to the present day. In fact, his Monte Carlo simulations in 1973 during his Ph.D. studies were apparently the very first molecular simulations carried out in the entire Soviet block of countries, and one of the first in the world on systems with orientation-dependent interactions. His contributions range from the fluctuating particle method for determining the chemical potential [27] and its implementation for Gibbs Ensemble simulations [28,29], to the very recent development of a new multi-particle-move Monte Carlo method [30,31]. He also collaborated with Bill and others on the development and implementation of the Reaction Ensemble Monte Carlo (REMC) simulation method to directly simulate the reaction and phase equilibrium compositions of multi-species systems [32–34].

Ivo's main activity since the 1990s has been in the modelling of polar and associating fluids, with special focus on water [25,35,36]. He has developed a new theoretical approach for perturbation theories, independent of the details of the underlying intermolecular interactions [37–43]. This approach, based on fundamental-level approximations that are aimed at capturing the essence of the interactions at short separation distances, promises to provide a simplified and useful approach for calculating the thermodynamic properties of complex fluids and their mixtures. This work was summarised in an invited review article [44] and in a 'Perspectives' paper [45]. In addition to his work on the behaviour of bulk fluids and mixtures, Ivo has also extended his interests to molecularly confined fluids [27,37] and, quite recently, to the phenomenon of electrospinning [46].

Ivo has supervised multiple graduate students and postdoctoral fellows through the years, many of whom have gone on to successful research careers. He has also collaborated with many colleagues, both in the Czech Republic and around the world, including his previous students and postdoctoral fellows. He has spent significant periods of time as a post-doc and visiting professor at universities overseas: 2 years in the United States (Rice University, Houston; University of Oklahoma, Norman; University of Tennessee, Knoxville), and altogether about 5 years with Bill as a visiting professor in Canada, first at the University of Guelph, and from 2004–2011 at the University of Ontario Institute of Technology in Oshawa.

Ivo has published more than 210 papers in international journals, which have achieved over 4000 citations, and he has an h-index of 34, one of the highest in the entire Czech physics community. His contributions to the development of molecular theories of fluids have also been acknowledged by several prestigious awards and nominations. He twice received the national award of the Board of Chemistry of the Czech Academy of Sciences, and in 1980 he was awarded the Prize of the Academy of Sciences, jointly with Tomáš Boublík. In 2004, he was the sole nominee of the Czech Republic for the prestigious Wolf Foundation Prize in chemistry, 'in recognition of his pioneering work in the theoretical modelling of complex fluids, and for his outstanding contributions to understanding the behaviour of liquids based on molecular principles'.

Carlos recalls: 'I first met Ivo in the spring of 1989, while I was on a three month stay in the University of Bochum with Prof. Johan Fischer. Ivo visited Johan for several weeks and we were lodged in the same residence. Since the residence was about a 30 minute walk from the University, we often returned to the residence together and

chatted all the way back. At one point I mentioned that every Wednesday there was a football match in the residence (playing on grass which, for a Spaniard like me, was a unique experience). He immediately decided to join the student group for the football match. At that time I did not know that Ivo, when younger, had played for Sparta Prague. When playing football (some people say with most things), Ivo becomes very competitive. I visited him in the autumn of 2013 (thus visiting Ústí for the first time) and he complained about the fact he must now play both soccer and tennis with much younger people, because most of the former colleagues he used to play with are not able to play any more. (I explained to him that this is not entirely unusual.)'

Ivo has two lovely daughters, Lenka and Sarka, who celebrated their 45th and 35th birthdays around the same time as Ivo's 70th. He also has four grandsons and two grand-daughters, with whom he tries to spend as much time as possible, in particular at his 200-year old farm house, located in a small village about 90 km south of Prague. With its internet connection, this is also a wonderful venue for doing his research in a quiet setting.

Ivo has no intention of retiring, and we expect that he will continue to be actively involved in scientific research in the statistical mechanics of fluids for years to come. We look forward to his continuing contributions.

3. The Liblice Conferences on the Statistical Mechanics of Liquids

A major contribution to fostering progress in the statistical mechanics of liquids has been Ivo's origination and continued coordination of the extremely successful Liblice Conference on the Statistical Mechanics of Liquids. Initiated in 1983, in part because although Czechoslovak scientists were not allowed to attend conferences abroad, hosting foreign scientists at conferences in Czechoslovakia was encouraged. It started on a modest scale, and meetings have been held every 4 years since 1986; they have grown into large international gatherings, attended by around 140 participants from all over the world. The name of the series is derived from the site where the first meeting was held, at the stately manor house called 'Liblice', the official congress centre of the Czechoslovak Academy of Sciences at the time. The first three conferences were officially organised under the auspices of the Chemical Physics Section of the Czechoslovak Chemical Society, and subsequent meetings have formally been organised jointly by the Academy of Sciences of the Czech Republic and Cornell University, represented by Ivo Nezbeda and Keith Gubbins, respectively. At each meeting, one is isolated in the middle of the Czech Republic, with an exceptional scientific programme, and with the real chance of having discussions and interactions with a lot of good scientists. The atmosphere at night is usually very good (the good Czech beer helps in creating a great atmosphere among liquid state theory physicists, and sometimes 'tequila' from Mexico via Fernando del Rio further improves the atmosphere.)

Bill attended the very first, and many of the subsequent, Liblice meetings. Carlos attended his first Liblice Conference in 1990 at Bechyne Castle, recalling it as 'an unforgettable experience'. At that time it was rather unusual to have scientists from Western and Eastern countries together in a conference, and a visa was needed to attend the first editions of the Liblice Conference. The Liblice Conference series has not been organised by any society/government. It has been simply due to Ivo's initiative (plus, obviously, the generous assistance of many of his co-workers). We can imagine that to obtain the permissions to organise such a conference has not been easy, particularly in the early years. One thing is for certain, Ivo was able to bring some of the most influential scientists working on liquid state theory to the conference to present and discuss the latest progress in the field. In that respect, a visit to the web page of the conference (http://liblice.icpf.cas.cz/) provides a flavour of the topics and the scientists that have participated over the years.

The Conference reflects Ivo's personality very well. Instructions like 'NO USE OF PRIVATE NOTEBOOK COMPUTERS WILL BE ALLOWED (OR POSSIBLE)' indicate clearly that you had better copy your lecture onto the main computer of the conference room in advance. With Ivo you know what is going on, he will let you know right away if your calculations are right/wrong, whether he likes your model/theory (or not). He maintains a high level of compromise when it comes to correct and rigorous results. Ivo shares some features with the patchy model that he developed in the 1980s. Although you may feel a hard-sphere repulsion at short distances, it is even more true that, when you approach in the right direction you feel a strong attractive square well. We like Ivo the way he is, and we admire his energy to do so many things and to lead so many projects. Soccer is probably not for soft people, and life probably not either.

As a leading figure in the Czech liquid matter community and a tireless organiser, Ivo regularly organises annual Czech workshops on liquid matter, often involving a small number of invited foreign speakers. These meetings provide an ideal opportunity for students, junior researchers and more senior scientists to meet together, exchange ideas and keep abreast of the latest developments in the field (and to enjoy the Czech tradition of performing unofficial experiments on liquid matter involving ethanol).

By means of the Liblice Conferences, Ivo, similarly as Tomáš, has been putting Czechoslovakia, and later the Czech Republic, on the scientific map. At this conference one can meet many of the people doing excellent science on liquids in this country (Kolafa, Labík, Lísal, Malijevsky, Předota, and many others). We are extremely grateful to Ivo

for organising this conference series over so many years, and we have now become a kind of family.

Ivo has been able to further develop the Czech School of Statistical Mechanics through his many former Ph.D. students and former collaborators, extending the path initiated by Tomáš. We have been fortunate enough to meet both of them, and to collaborate and to publish with both. We are well aware that doing good science is not easy when undertaken in difficult times. In Spain, although for other reasons, similar difficulties were faced over the past century. We think Tomáš, Ivo and many others from the Czech School of Statistical Mechanics have done excellent work.

4. Summary and outlook

We are pleased to have this special issue in memory of Tomáš Boublík and in honour of Ivo Nezbeda's 70th birthday appear in Molecular Physics, in which they both published so many papers. It contains about 30 interesting papers from different countries dealing with various aspects of the statistical mechanics of liquids. We are sure that all of the authors and co-authors of this issue join with us in extending our best wishes to Ivo on the occasion of his birthday, and in celebrating the scientific achievements of Tomáš.

Tomáš and Ivo wrote what is probably the best existing review paper dealing with the EOS of hard bodies [3]. Hard-body systems are not only important because they can be used as reference systems when developing perturbation theories for molecular fluids, but interest in them as a model system has recently arisen from an entirely different community, that of colloidal chemistry. For example, it is now possible to synthesise colloidal particles whose effective interaction is well described by a hard potential. Thus, the colloidal realisation of 'hard spheres', 'hard dumbbells' and many other shapes is now possible. Furthermore, 'patchy colloids' can be modelled by extensions of the Smith–Nezbeda model of associating fluids [22]. We are sure that this community will benefit from all the knowledge developed by Tomáš and Ivo, and that their works will continue to be cited well into the future, both in the field of colloidal chemistry and in many other areas.

Disclosure statement

No potential conflict of interest was reported by the authors.

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