

STRUCTURAL CHEMISTRY INDABA II

INTERMOLECULAR INTERACTIONS

3-8 August 1997 : Kruger National Park, South Africa

An international workshop organized by the South African Crystallographic Society in collaboration with the Commission on Structural Chemistry of the International Union of Crystallography.

IUCr Scientific Freedom Policy Statement:

The Organising Committee of the Structural Chemistry Indaba shall observe the basic policy of non discrimination and affirms the rights of scientists throughout the world to adhere to or to associate with international scientific activity without restrictions based on nationality, race, colour, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes of the International Council of Scientific Unions. At this conference no barriers will exist which would prevent the participation of bona fide scientists.

Indaba is an African term to describe a meeting to analyze a difficult problem from all angles

THEME - Intermolecular Interactions

Each of the invited lecturers will address a different aspect around the central theme of Intermolecular Interactions, starting with a critical overview of the assumptions common amongst structural chemists.

The idea of intermolecular interactions relates to the notion that materials in the bulk consist of weakly interacting units, or molecules, in the sense that intramolecular interactions are stronger than these, by orders of magnitude. In view of this it is argued that, by ignoring the weak interactions, the same molecular units that occur in the gas phase can be recognized in condensed phases. At the same time it is commonly accepted that solid materials exhibit many properties not apparent in other phases and acquired as a result of intermolecular interactions only. From both points of view the concept is rather ill-defined and of questionable importance. The problem relates to the model of choice to describe condensed phases. Defined as single quantum-mechanical systems there is no basis to distinguish between intra- and intermolecular forces. An intermolecular interaction is then defined only for the gas phase, where it is practically negligible in any case.

An attempt to distinguish between intra- and intermolecular interactions necessarily fails to recognize their interdependence and creates artifacts to be used later on as independent concepts, in terms of which to explain chemical behavior. In terms of deformation electron densities in crystals the distinction becomes even more vague and the definition of molecular units even more arbitrary.

Answers to these questions are probably not simple and different points of view can surely be formulated in all cases.

In this sense it provides a worthy topic for discussion at a special symposium in the spirit of the 1995 Small-molecules Indaba.

INVITED LECTURERS

Note: This is a preliminary list. Some still have to be confirmed and one or two more lecturers may still be invited.

Name	From	Topic
F.H.Allen	Cambridge, UK	The relationship between theory and experiment in the study of non-covalent interactions.
A.Amann	ETH, Switzerland	The shape of interacting molecules
I.Bernal	Houston, USA	Conglomerate Crystallization.
J.C.A.Boeyens	Witwatersrand, South Africa	Intermolecular Bonding
D.Braga	Bologna, Italy	Supramolecular organization in organometallic crystals.
P.Comba	Heidelberg, Germany	Intermolecular effects in coordination chemistry.
T.Cundari	Memphis, USA	Modeling intermolecular effects
G.Gilli	Ferrara, Italy	Strong interactions (or incipient interactions) in molecular crystals: an implicit criticism of the inter-intramolecular dichotomy.
J.A.K.Howard	Durham, UK	Intermolecular effects at 10K.
C.Krueger	MPI, Germany	Electron deformation densities.
T.Koritsanszky	Berlin, Germany	Electron densities between molecules.
P.Luger	Berlin, Germany	Interactions at low temperatures.
J.Ogilvie	Oregon, USA	Dynamic aspects of intermolecular interactions.
A.G.Orpen	Bristol, UK	Structural evidence of intermolecular interactions.
E.Osawa	Japan	Design of Crystal Properties.
D.Rouvray	UK	Fuzzy logic applied to the molecular sphere.
B.T.Sutcliffe	York, UK	Molecular properties in different environments.

VENUE

As with the Conference in August 1995, the second Indaba will be held in one of the most famous national parks in the world and the oldest one in Africa, the Kruger National Park. The same venue as before, the picturesque Skukuza camp, has been secured for the duration of the workshop.

One of the Park's main objectives is to maintain the ecosystem in its natural state and to offer the visitor an unrivaled experience of African wildlife.

While offering excellent accommodation facilities, the Park has retained a genuine African atmosphere - to the delight of the scores of visitors to the New South Africa.

The climate is subtropical, with days normally sunny, warm and clear. During August, just before the onset of the warm African summer, the temperatures are moderate and pleasant. In this regard the South African author and nature lover, C.Louis Leipoldt, wrote: "The ideal time to visit the Bushveld is in winter, from May to November. Then the climate is charmingly even: its mornings, when the sun tinges the tops of the bush, are delightfully crisp and cool; its noon is pleasantly but not relaxingly warm; its afternoons and evenings, stained by an all-too-brief afterglow with amazingly vivid colouring, are as mild and beautiful as a summer's night in Europe".

Excursions into the Park will give both delegates and accompanying persons many opportunities to view the unparalleled diversity of wildlife, including antelope, buffalo, elephant, lion, leopard, cheetah, wild dog, hyena, jackal, black and white rhinoceros, an exceptional variety of bird species and numerous other wild creatures. Skukuza is the Kruger Park's main camp. Dress code: Casual.

COST

Final Pricing

Registration fee	includes admittance to all scientific sessions, the Book of Abstracts, the meet and greet party on Sunday, the traditional braai, a daily finger buffet breakfast and teas, as well as daily excursions into the park	\$330
Early registration	payment must be received before April 15, 1997	\$280
Student registration	For subsidised students	\$100
Accompanying persons registration fee	includes only the traditional braai and daily excursions into the park	\$100
Transport between the airport and Skukuza camp	includes entrance fee into Kruger Park	\$100
Banquet	a traditional dinner to be held on Tuesday 5th	\$30

Note:

- The above costs do NOT include accommodation costs nor meals not explicitly included above.
- The daily finger breakfast buffet will be provided at the lecture hall, as will the teas.
- The camp has restaurant facilities for normal meals, breakfast, lunch and supper, with prices ranging from \$5 to \$12.
- People making their own way to the park will have to pay for the park entrance at the gate (about \$15 per car and \$4 per person..).
- PLEASE NOTE: The number of participants is restricted due to limitations in accommodation at Skukuza camp. PLEASE BOOK EARLY.

TRANSPORT

Johannesburg International Airport is well utilized by many major airlines from Europe, America and most other parts of the world. Normally trips from Europe last over 12 hours and are undertaken overnight, so leaving on the evening of Saturday the 2nd of August will allow you to arrive at JIA on Sunday the 3rd. Flights leaving JIA on the evening of Friday 8th August will arrive in Europe on the morning of Saturday 9th.

Travelers from Europe will feel no jet lag, but the Americas are 6 to 9 hours behind South Africa, while Asia is 2 to 10 hours ahead.

Visas may be required for some countries. Please make all travel arrangements with your local travel agents, but inform us of your arrival date, time, flight number etc.

Coach

Transport from the airport to the Skukuza camp in the Kruger National Park will be provided by coach for those that require it, at a cost of \$100 per person. The bus trip will include refreshments and orientation information. For accompanying persons, and conference attendees, the bus will remain available for daily excursions into the park for the duration of the conference. The use of the bus for these excursions is included in the registration fee. The full bus fare is for the trips to and from the airport on the 3rd and 8th. Preliminary dates are:

JIA to Skukuza	morning of 3rd August
Park outings	afternoons of 3rd to 7th August
Skukuza to JIA	afternoon of 8th August

Car Rental

Many international car rental companies (Avis, Hertz, Budget, etc.) are represented in South Africa. Attendees wishing to rent cars should apply through their local travel agents.

ACCOMMODATION

Accommodation available at Skukuza camp is in typical national park style. The rondawels are individual huts with hot and cold running water, linen service, and full ablation facilities. The number of beds per rondawel ranges from 2 to 6. To facilitate bookings the accommodation has been grouped into three categories.

The following prices are per person per night:

category	price pp pn	deposit
luxury (single)	\$60.00	\$150.00
standard (sharing)	\$30.00	\$75.00
basic (sharing)	\$25.00	\$65.00

- Please indicate your order of preference on the registration form
- Families or groups wishing to stay together must contact us well in advance to ensure booking of appropriate accommodation. Prices for such arrangements will depend on final availability.
- Because the accommodation capacity within each category varies, it is impossible to guarantee a specific allocation. We will, however, try our best to meet your specific requirements.
- Accommodation will be allocated on a first come, first served basis.
- or shared accommodation, please indicate any partner preferences.
- The required deposit must be received by 31st June 1997 and will contribute towards the full accommodation cost, the balance of which can be settled on arrival.

REGISTRATION AND SUBMISSION OF ABSTRACTS

Deadlines		Cancellation Penalties	
early bird registration	15th April 1997	before 31st July	50%
final registration	15 June 1997	after 31st July	no refund
final payments due	31 June 1997		
submission of abstracts	31 June 1997		

Registration

A registration form is available on the WWW at <http://www.gh.wits.ac.za/indaba/reg-indaba.html>. This form can be used for preliminary registration to book a place at the indaba. If you would prefer to fax the registration form, you may do so by either printing the WWW page, or by using the text only page at <http://www.gh.wits.ac.za/indaba/reg-indaba.txt>. This text only page is also ideal for emailing your registration to the primary contact email address below.

Payment

There are two preferred methods of payment

- Direct bank transfer into the bank account: "Structural Chemistry Indaba" Account number 1951076273 NedBank, Johannesburg. Wits branch 19510502 SOUTH AFRICA
- Cheque or bank draft made payable to the above account and mailed to the primary registration mail address below.

Please also contact us via email, fax or mail when you make the transfer, so that we have our own record of the payments. If you would prefer to pay with a credit card, arrangements can be made, but a surcharge of 6% will be charged.

Submission of Abstracts

Submission of abstracts can be made by mail, email or ftp. If using mail or email, please post to the primary contact address below. If using ftp please ftp into the anonymous ftp account at <ftp://www.gh.wits.ac.za/indaba>. Electronic submission of abstracts will be accepted in the following formats only:

- Plain text (ASCII)
- Postscript
- TeX and LaTeX
- WPS.1 and WP6.0 for DOS or Windows (not Macintosh)
- Word2.0 for Windows (not Macintosh)

All these formats will be accepted for ftp submissions. For email submissions, the plain text, TeX, LaTeX and postscript files can be sent in the body of the email or as attachments, while the WP and Word files must be sent as attachments, apologies, but Macintosh attachments can NOT be accepted. If you are using a Macintosh email program, please only use the text formats (plain text, postscript, TeX or LaTeX) and include the submission in the body of the mail.

Note that since the number of participants will be limited, and interest in the conference is high, early registration is very advisable.

CONTACTS

The primary means of contacting the organizers for information, registration, and submission of abstracts will be through the e-mail address:

indaba-org@hobbes.gh.wits.ac.za

This address is guaranteed to reach the person most likely to be in a position to answer any questions you might have, or provide the information you are looking for.

The primary telephone, fax and mail address for submission of registration, abstracts and payment by cheque or bank draft is to the Conference organizer's address below:

Conference Organiser

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