Honourable Rector Magnificus,
Members of the University Community,
Ladies and Gentlemen.

First of all let me say how honoured and extremely grateful I am to the University of Murcia for bestowing upon me the Honorary Doctorate. I accept it joyfully both for myself and also on behalf of all the people with whom I have worked for the last 30 years. I have been very fortunate to attract several excellent Spanish postdoctoral researchers to my group, some of whom are present today: David Curiel, Antonio Caballero and Fabiola Zapata.

My research career began with a PhD (1979-1982) in the area of organophosphorus chemistry under the supervision of Dr Dennis Hall at King's College, University of London. A Royal Society European postdoctoral fellowship (1982-1983) enabled me to change research direction and conduct research in supramolecular chemistry with Professor Jean-Marie Lehn at the Universite Louis Pasteur, Strasbourg, France. After a demonstratorship, which is a temporary lectureship, at the University of Exeter (1983-1984) I took up a Lectureship at the University of Birmingham in 1984. In 1990 I moved to the Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, and became a Fellow of Wadham College Oxford. Since 1998 I have been a Professor.

I will now attempt to describe my work in as clear and straightforward

way as I can.

Over the past three decades, my research group has made major contributions to the general field of host-guest chemistry, which has its historical origins dating back to Emil Fisher's 1894 famous lock (host) and key (guest) analogy. The design and construction of new host systems that are capable of discriminating between a number of different guests is the basis for what is called 'molecular recognition'. It is one of the key growth areas in chemistry, adding to the fundamental knowledge of how one molecule recognises and interacts with another molecule. My research group is known for combining molecular recognition with sensing, where a 'light bulb' attached to the periphery of the host is 'switched on' only when a target guest matches the geometric shape and size of the host's cavity. In particular, we have constructed a variety of elaborate host molecules including ring shaped and chain-like interlocked systems containing 'light-bulb' reporter groups. These can recognise and sense positively charged (cationic) and negatively charged (anionic) guest species, such as positive sodium cations and negative chloride anions.

During the first decade of my independent academic career (mid-1980's to mid-1990's) the research interests of my group focused on developing electrochemical sensors for positively charged cations such as sodium, potassium and ammonium. An electro-chemical probe, known as ferrocene (which is like an iron atom, sandwiched between two five-membered carbon rings), was integrated into various carbon-oxygen ring shaped hosts, known as crown ethers. Upon cation guest binding in the centre of the crown ether, the nearby ferrocene probe detected its presence with an electro-chemical response. Having demonstrated the principle of 'electrochemical molecular recognition' for positively charged guest species, we turned our attention to extending this to negatively charged guests.

Negatively charged species, anions, are everywhere in the natural world and play fundamental roles in many biological, environmental and medical processes. For example the molecule of life, DNA, is a polyanion. The overuse of fertilisers in arable farming has resulted in phosphate and nitrate contaminants in lakes and rivers leading to algal blooms disrupting aquatic life cycles. Anion dysregulation is linked to several physiological diseases such as cystic fibrosis. In spite of this, surprisingly, at the beginning of the 1990s the field of designing hosts for anions was still in its infancy. Nature recognises anions using positively charged entities and 'hydrogen bonding'. Hydrogen bonding is where a hydrogen atom with positive character forms an attractive interaction (bond) with a negative atom. Hydrogen bonding is responsible for the high boiling point of water. We used a positively charged electrochemical probe, called cobaltocenium and ferrocene hydrogen bonding

hosts to sense anionic guest species using electrochemical methods. We subsequently developed a series of transition metal cyclic hosts capable of sensing anions using both electrochemical and luminescence methods.

We then wanted to improve upon our 'Mark 1' hosts to design 'Mark 2' host systems for anions. And we used mechanically interlocked molecules to do this.

A rotaxane, from the Latin words rota (wheel) and axis (axle) is a mechanically interlocked molecule which comprises a ring threaded by a rod-like axle with stopper endgroups (like a dumb bell). A catenane, derived from the Latin word catena (chain) is another mechanically interlocked molecule which has two or more interlocking ring shaped component parts. At the beginning of this century we started to design both rotaxane and catenane structures to contain unique three dimensional cavities for recognising anions. We pioneered the synthesis of such interlocked host structures using anions to bring together ('template') the separate components. This involved threading a molecular component through the circular cavity of a ring. The ring is called a macrocycle. It is like passing a thread through the eye of a needle. The work led to using a chloride anion to template the first rotaxane and catenane interlocked host molecules. After removing the template the resulting interlocked cavity displayed a high degree of selectivity for chloride. This was in preference to phosphate and nitrate, which are too large to penetrate the binding pocket. The methodology was further demonstrated with bromide, sulfate, nitrate and nitrite anion templates for the synthesis of a range of interlocked host structures. Most importantly, the 'Mark 2' interlocked hosts displayed far superior levels of anion recognition compared to 'Mark 1' non-interlocked host systems.

We subsequently began to incorporate 'light bulbs' into these structures in an effort to combine the superior level of recognition of these interlocked hosts with sensing capability. 'Light bulbs', such as certain transition metal and lanthanide metal luminophores, integrated into either macrocyclic or axle components of rotaxanes exhibited selective optical sensing of anions. Our first work in this area, around 2005, incorporated luminescent transition metal 'light bulbs' into rotaxane hosts. Such a host, prepared by David Curiel, selectively recognised and sensed, via luminescence, a hydrogen sulphate anion.

In the last few years we have been exploiting another attractive interaction called ‘halogen bonding’. Halogen bonding is the interaction between polarised halogen atoms of positive character and electron rich neutral or anionic species. It is similar to hydrogen bonding with the hydrogen atom replaced by a halogen atom, such as iodine. Of the many attractive

interactions commonly used in molecular recognition, halogen bonding is the least exploited. In a significant step forward, we demonstrated the first examples of halogen bonding hosts to recognise anions in aqueous media, and to facilitate the anion template assembly of interlocked structures. Most importantly, the incorporation of halogen bond donors into ring shaped cyclic and interlocked hosts dramatically influenced anion selectivity and enhanced anion recognition capability compared to hydrogen bonding hosts. For example a family of fluorescent cyclic and catenane hosts selectively sensed chloride, bromide and iodide anions. Antonio Caballero and Fabiola Zapata were the researchers involved in this work. Importantly, in a recent major development we have demonstrated the superiority of halogen bonding over hydrogen bonding as an attractive interaction for anion binding in water.

The potential for mechanically interlocked molecules to act as molecular "machines" was highlighted by the 2016 Nobel Prize in Chemistry. Our current work is developing materials which can be thought of as "molecular machine-like sensors".

I hope the fundamental research contributed by my group will have long-term impact upon monitoring the environment, on personalized healthcare and diagnostic medicine.

Thomas Aquinas told us that "there is nothing on this earth more to be prized than true friendship." And I am grateful for the academic friendships that transcend borders and distances, for the friendships that allow us jointly to explore the world in which we live, and for the friendships that enable us to share together in our successes. Thank you for this honour. Thank you, my friends.


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Ceremonia de Investidura del
Profesor Dr. Paul D. Beer
La Opinión DE MURCIA


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