Quantum Conversations & the Art of Fluorescence

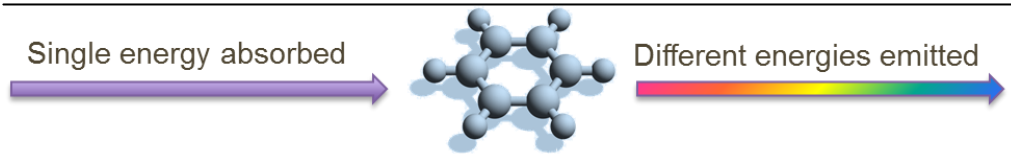
Patterns in Nature ~ The Hidden World of Molecules

Images from the Laser Spectroscopy and Molecular Dynamics Laboratory in the School of Chemical and Physical Sciences, Flinders University where the molecules are the artists.

Experimental images are obtained using a world class instrument built at Flinders University. Calculated images are generated to try and match the experimental observations. From this, we learn about a molecule's shape.

The images are maps of the energies within a molecule. They tell us how it rotates and vibrates.

The images can be thought of as a "conversation" with a molecule. The molecule is asked a "question" by exposing it to laser light of a known energy. The molecule may absorb this light and "answers" by emitting its own light, but at differing energies. By recording the answers (emitted energies) to different questions (different probe energies) a map of the conversation is built up.



Although the images are a direct consequence of Quantum Physics, they can be appreciated simply for their patterns and symmetry.

The laboratory is a training ground for future researchers, and regularly trains students in experimental science. Where an image has been recorded by a student we have credited them with the work.

We hope you enjoy the images on display, and urge you to look closely at the images to discover underlying patterns for yourself.

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By observing the energies of light that are absorbed, and measuring the energies of light that are emitted, an energy map is produced that is a "fingerprint" of the molecule's molecular motion.

1. Fluorobenzene - Comet

Experimental observation of fluorobenzene at 298 K (25 °C)
Recorded: March 28, 2010

This image was the first published image from our laboratory using the apparatus. It was recorded since we found that experiments performed in the 1970's did not determine the fluorobenzene rotational energy levels correctly. Our 2-dimensional technique clearly showed the previous values to be wrong and we were able to provide higher precision values.

Inspiration for displaying our work as an exhibition came from comments by an assessor reviewing our manuscript. The reviewer stated "some of the figures could be art!".

The image contains multiple "comets" along the diagonal. The features observed within each of the comets are due to quantised rotations and rules governing changes between them. The different comets arise from fluorobenzene molecules that vibrate in different ways. Very weak comets can be seen away from the diagonal line which denote molecules that have started in one type of vibration and, after interrogation, have finished in a different vibration.

These results were published in *The Journal of Chemical Physics,* Volume 134, Article Number 184301, 2011.

2. Fluorobenzene - Peacock

Calculated image of fluorobenzene at 298 K (25 °C)

Calculated images are important for understanding those recorded experimentally. We calculated this image to understand and assign the structure seen in our experimental fluorobenzene image. Although the image is calculated at a much higher resolution than our instrument could ever record, it allows us to precisely determine the changes that occur in the way the molecule rotates during the interrogation.

Many different patterns exist in the image. Both from a visual perspective and a quantum physics point of view there are a number of different ways in which it is possible to "connect the dots".

Each dot on the image corresponds to a "conversation" with a fluorobenzene molecule. Where they occur is determined by the molecule's starting rotational motion, the rotational motion after the laser hits it, and the final rotational motion following emission of light.

Several small sections from this image were printed in grey scale in *The Journal of Chemical Physics,* Volume 134, article number 184301, 2011.

3. Benzene - Firebird

Experimental observation of fluorobenzene at 298 K (25 °C)
Recorded: March 25, 2010 ~ Student Experimenter: Olivia Maselli

Benzene molecules show a different characteristic pattern when compared to fluorobenzene. Within this image there are different patterns, including a bird shaped pattern, due to different vibrational motions of the benzene molecules.

This image was recorded to solve a specific problem due to the complex nature of benzene vibrations that are close in energy and thus hard to see individually. The stack of multiple diagonal lines are due to different vibrational motions of the molecule. The 2D image allows us to tease apart the different vibrations giving us a better chance at solving the problem.

4. Fluorobenzene - Checker

Calculated image of fluorobenzene at 298 K (25 °C)

Colour or lack of colour plays a role in image analysis as patterns and intensities are compared. Exploring the abundant detail in the calculated fluorobenzene rotational energy pattern can be aided by varying between colour, black on white and white on black. The display shows repeated images that are rotated and, since there no correct orientation to display the images, each is equally valid.

5. Fluorobenzene - Stars

Experimental observation of fluorobenzene at 7 K (-266 °C), near absolute zero.
Recorded: February 7, 2012

Cooling molecules reduces their available energy, thus eliminating high energy vibrations and rotations, and allows different features to be revealed. Weaker “stars” are due to the naturally occurring isotope carbon 13 replacing a carbon 12 atom in the fluorobenzene molecule. This subtle change in mass is seen as a weaker pattern shifted in energy compared to the brighter all-carbon-12 “stars”.

Cold temperatures also allow molecules to stick together and form “clusters” that would otherwise fall apart. There is in fact a weak bright spot due to fluorobenzene weakly bound to an argon atom. This fluorobenzene-argon cluster does not have the usual star shape due to the change in the molecule’s shape. The 2D image allows us to survey the “landscape” for the signatures of different molecular species in our field of view.

6. Phenol - Wings

Experimental observation of phenol at 298 K (25 °C)
Recorded: April 5, 2012 ~ Student Experimenter: Abdullah Alsubaie

As with all of the images in this collection, it can be viewed either horizontally or vertically. This image was the result of an investigation into an apparent discrepancy in the existing literature dating from the 1970's. In applying our technique to this problem, this experimental image was acquired as a "first attempt". It contains experimental artefacts (the horizontal and vertical intersecting bands) due to the phenol molecules reabsorbing the emitted light before it could reach the detector. There are, however, enough other detailed features in this image to provide a test of the calculated image. We found that no more experiments were needed since experiment and calculation agreed and the most recent determinations of energy values are reliable.

This is an example of experimental work where significant effort went in to recording the image but the results don't warrant reporting in the scientific literature for its own sake.

7. Fluorobenzene - Symphony

Calculated image of fluorobenzene at 298 K (25 °C)

A close - up view of the overall calculated energy pattern for fluorobenzene reveals overlaid ordered patterns. Each dot corresponds to an allowed energy change in the molecule, with the negative space corresponding to a forbidden energy. The apparent chaos of the patterns when we view a wider section of the overall fluorobenzene image is reduced here to reveal quite ordered structure underlying the chaos. There is a balance of chaos and harmony reminiscent of multiple musical instruments being played at once in a symphony.

8. Fluorobenzene - Fire & Ice

Calculated image of fluorobenzene at 298 K (25 °C)

A close - up section of the calculated fluorobenzene energy patterns showing that the 2D technique can be used with commercially available instruments to produce suitably detailed results in other labs.

9. Fluorobenzene - Cool

Calculated image of fluorobenzene from 298 K (25 °C) to 7K (-266°C)

This image uses the calculated fluorobenzene energy pattern to show how the pattern is condensed as the molecules are cooled from room temperature to near absolute zero. The experimental apparatus cools the sample gas down to very low temperatures so that by the time the sample molecules intersect with the laser, they have reduced their rotational and vibrational energy significantly.

The cooling is a result of forcing high pressure gas through a small hole in a vacuum chamber. It reduces the congestion of overlapping features. Cooling also allows molecules to cling together so that weakly bound clusters can be studied. Weak, but very important, forces that link molecules together can thus be studied. These weak forces are important in determining structure of large, complex molecules such as proteins.

10. Hydroxyl - Stack (large)

Experimental observation of the hydroxyl radical, (OH) at 893K (620 °C)
Recorded: December 2, 2009 ~ Student Experimenter: Amelia Gontar

A simpler energy pattern emerges from a molecule made up of only two atoms—oxygen (O) and hydrogen (H). The hydroxyl radical (OH) is a key species in the atmosphere.

The “stripes” show the images seen by the detector as it records the emitted light spread out into its component energies. Images such as these are collected at each new laser energy input into the OH molecules. These images form stage 1 of the imaging process. Stage 2 is shown by the raised “dashed” 2D image. The yellow striped image forms one slice of the dashed image. Specifically it is condensed down to form the yellow section of the dashed image. Likewise, the light blue striped image is condensed to form the light blue section of the dashed image.

This “colour coding” of these images is different to the colouring technique used in other 2D images where the colour gradient and contrast is used as an aid to data analysis.

11. Fluorobenzene - Fireworks

Calculated image of fluorobenzene at 7K (-266 °C), near absolute zero.

For the calculation, the energy available to the molecule for rotating has been limited by limiting the temperature. The flare or comet shape is reduced to a more compact shape. Allowed energy changes are indicated by the dots in the image.

12. Toluene- Launch

Experimental observation of toluene at 298 K (25 °C).
Recorded: June 10, 2012

Areas of light and no light with a strong drop off between each region.
The light emitted from toluene molecules, as captured by our apparatus after they have absorbed laser light reveals a similar yet different pattern to light from fluorobenzene.

This image also illustrates the development of the image analysis software in tandem with the experimental apparatus. As less intense features such as those in the dark region of this image appear, the software architecture is adjusted accordingly to maximise the imaging ability for weak features in the images.

13. Fluorobenzene - Arch

Calculated image of fluorobenzene at 298 K (25 °C).

This image shows a more dramatic contrast of the item 2 clearly showing the quantum nature of molecules. The dots represent the allowed energy states and the voids represent energies that the molecule does not respond to. This is showing the quantisation of the molecule's energy.

Many different patterns exist in the image. Both from a visual perspective and a quantum physics point of view there are a number of different ways in which it is possible to "connect the dots".

14. Water - Snowflake

Calculated image of water at 673K (400°C).

Water—the chemical of life—has a unique energy pattern. Here it is repeated and rotated, forming a snow flake pattern. The water molecule with its 3 atoms has an energy pattern complexity between that of the smaller hydroxyl radical (item 10) and the larger molecules (for example in item 13).

15. Fluorobenzene - Peacock Head

Calculated image of fluorobenzene at 298 K (25 °C).

This image shows a closer view of the larger image in item 2 with a slightly changed colour scheme to highlight a different view of the complex calculated pattern. Calculated images are important for understanding those recorded experimentally.

16. Hydroxyl - Stack (small)

Experimental observation of the hydroxyl radical, (OH) at 893K (620 °C)
Recorded: December 2, 2009 ~ Student Experimenter: Amelia Gontar

This is a reduced version of the larger hydroxyl stack (item 10). It draws ones attention to more the signal (coloured areas) and less of the natural noise associated with acquiring the images. Noise is seen as random, low intensity, uncoloured pixels scattered throughout the image. Noise is a constant part of experimental data acquisition and the challenge of experimental design and execution is to maximise signal and to minimise background noise.

17. Fluorobenzene - Stars (narrow)

Experimental observation of fluorobenzene at 7K (-266 °C), near absolute zero.
Recorded: February 7, 2012

This version of item 5 focuses only on the fluorobenzene patterns with the small van der Waals (weakly bound) fluorobenzene-argon cluster removed.

Molecules in Motion

What is a Molecule?

Molecules are atoms bound together. The atoms in the molecule have a 3-dimensional arrangement that is determined by the laws of physics.

Tumbling, Spinning, Rotating

Isolated molecules are free to rotate in 3-Dimensions.

What Keeps a Molecule Together?

Electrons are the glue of a molecule. They are shared between atoms to "bond" them together.

Springy Bonds

Atoms in a molecule jiggle about. The bonds between atoms act as springs. The atoms vibrate in a number of coordinated "dances".

Quantum Physics

Rules for the Tiny

The laws of physics for *small* things are different to those we experience in our *big* everyday world.

Quantisation

Quantum Physics often restricts a physical property (such as vibrations or rotations) to certain values—not all values are possible! The values are *Quantised*.

Strange Effects

Quantum Physics reveals several strange concepts that are very different to everyday experience. However, these concepts are predicted mathematically and shown experimentally.

Rules for Changes

If a physical property is quantised, then there can be rules about what changes are possible. These are *Selection Rules*.

Quantised Molecules

Vibrations

Atoms within a molecule must vibrate in a choreographed fashioned as directed by Quantum Physics.

There are only a limited number of *vibrational motions*; this is governed by the number of atoms.

A molecule can only vibrate with specific amounts, or *quanta,* of a vibrational motion.

Vibrational energy is quantised.

When is zero not zero?

Atoms in a molecule can never stop moving. The lowest vibrational energy possible in the molecule still requires the molecule to vibrate—called *Zero Point Energy*.

Rotations

The entire molecule can rotate in space, but only in a way that satisfies the laws of Quantum Physics.

A molecule can only rotate with specific amounts, or *quanta,* of a rotational motion.

Rotational energy is quantised.

Excited Molecules

A molecule not rotating and at its lowest vibrational energy is said to be in its *Ground State*. Otherwise, it is called *Excited* or in an *Excited State*.

Interacting with Light

Particles of Light

Light is made up of small packets of energy called *photons*.

Each photon has a fixed energy. In the visible spectrum, red photons have low energy, whilst violet photons have high energy.

Absorption of a photon increases a molecule's energy.

Release of a photon (called *fluorescence*) lowers a molecule's energy.

A Change of Motion

When molecules absorb or release light (a photon) they can change their rotational energy. They may also change to a different vibrational type and energy.

Quantisation of molecular motion means that only certain energy changes can occur within the molecule.

Incoming and outgoing photon energies must match the energy gaps in the molecule.

"The important thing in science is not so much to obtain new facts as to discover new ways of thinking about them."

- Sir William Lawrence Bragg, Australian-born physicist and recipient of the Nobel Prize for Physics in 1915 at the age of 25

(*via Australian Science Illustrated as noted on the RIAus Facebook page*)

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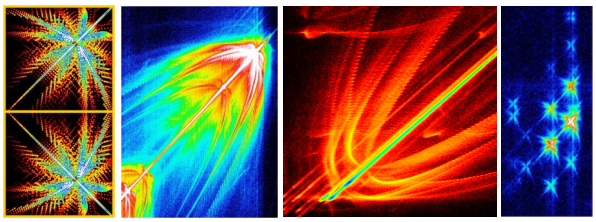

July 29 - Sept 2 for SALA 2012

Patterns in nature on the molecular level as seen by the Laser Lab, Flinders University.

Images obtained from a "conversation" with molecules through their interaction with light can be understood using quantum physics but they can also be viewed purely for their natural harmony and symmetry.

Visit: www.salainc.com.au/artist-portfolio.aspx?artistid=819

July 29 – Sept 2 for South Australian Living Artists Festival 2012
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Visit www.TheArtisanCafe.com.au for opening hours.