

## NMR spectroscopy without the 'M'

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[Pacific Northwest National Laboratory's NMR spectrometer](#)

Nuclear magnetic resonance (NMR) spectroscopy is perhaps the most useful technique in the organic chemist's toolkit. But conventional NMR requires the sample to be placed in a very high magnetic field, which needs large and expensive superconducting magnets cooled by liquid helium. Now, an interdisciplinary group in the US has managed to accomplish NMR spectroscopy without magnets. The work could lead to portable NMR spectrometers, and possibly even small personalized spectrometers for medical diagnosis.

### How it's done

The applied magnetic field serves several purposes in NMR. Most nuclei of interest in NMR

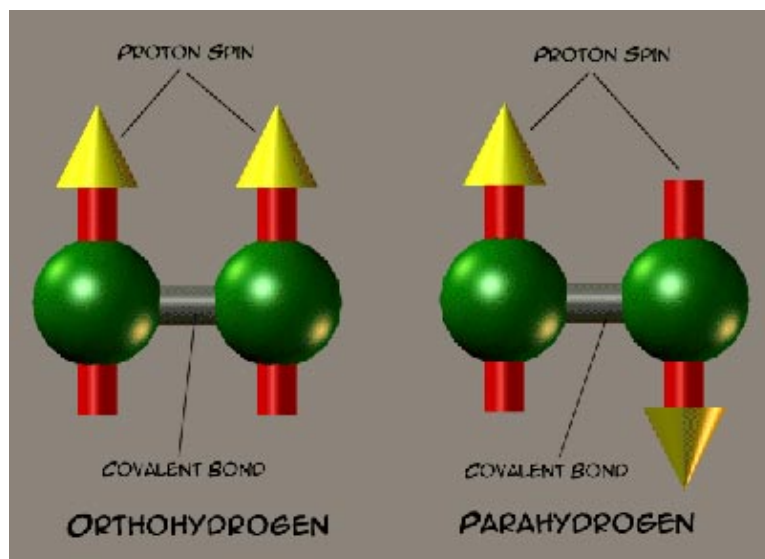
have two states – spin-up and spin-down. When placed in a magnetic field, the spin-down state is at a higher energy level than the spin-up state. Conventional NMR works by bombarding the sample with radio waves and measuring the energy absorbed or emitted when nuclei flip between the two states. The same nuclei in different parts of a molecule have slightly different transition frequencies; so measuring these frequencies allows researchers to work out the location of particular atoms in the molecule.

The bigger the magnetic field, the easier it is to resolve these different frequencies, providing a better understanding of complex molecules. Furthermore, a larger magnetic field increases the proportion of nuclei that are spin-up, which in turn causes a larger perturbation between the states, which gives a stronger signal.

The bottom line is that the signal intensity in conventional NMR increases roughly as the square of the magnetic field strength. NMR spectrometers over the years have therefore become bigger, more powerful and more expensive. The alternative – NMR spectroscopy with no applied field – seems bizarre because it should mean no energy gap, no spin polarization and nothing to measure.

## Spin couples

Fortunately, in addition to interacting with the magnetic field, the nuclear spins also interact with each other. This effect, called "J-coupling" or "spin-spin coupling" is much smaller, but it is still seen in a standard NMR spectrum as a splitting of the main absorption peaks. In the absence of an applied field, the J-coupling is all that remains. The researchers say that the signals resulting from pure J-coupling can impart plenty of information regarding chemical structure. "We have acquired zero-field J-spectra in dozens of molecules, and no two molecules have produced the same features," says atomic physicist Micah Ledbetter of the Nuclear Science Division at the University of California at Berkeley, who was part of the research. Nevertheless, since J-coupling is much weaker than the coupling to a strong applied field, the resonance associated with pure J-coupling is much harder to detect.



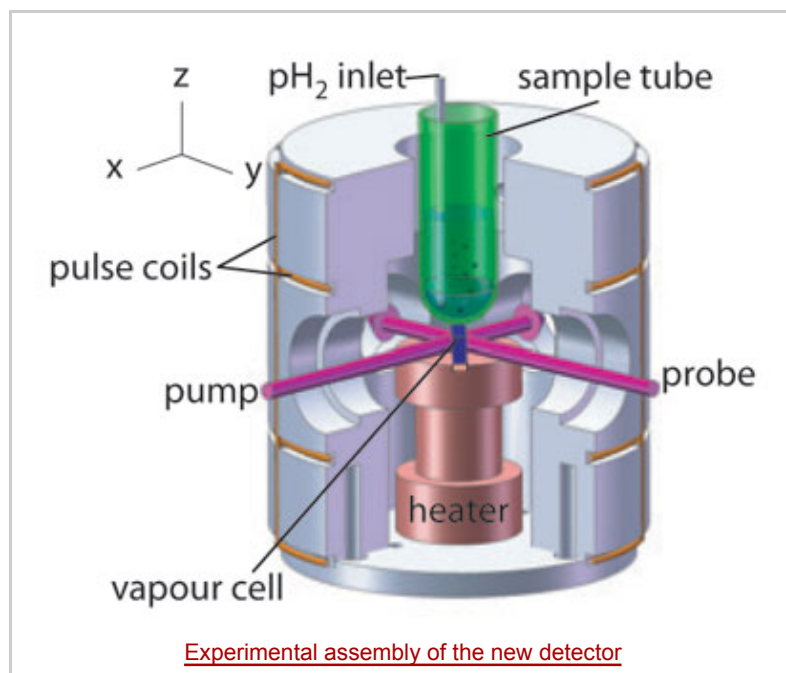
[Spin isomers of molecular hydrogen](#)

## Solve and resolve

The current research at Berkeley builds on previous work in low and zero-field NMR and attacks this problem in two ways. First, the problem of spin coupling without an applied magnetic field can be overcome by employing a technique known as "parahydrogen-induced polarization". Parahydrogen is a spin isomer form of hydrogen with the anti-parallel spin alignment, forming a "singlet state" (see image above). The technique used by them transfers a special kind of polarization from the sample molecule, resulting in enormous signal enhancement. While the phenomenon of parahydrogen-induced polarization has been known for some time, the current work is the first to successfully use it in zero-field.

The researchers then used an innovative technique to measure the faint magnetic fields. The detectors used in early experiments with low-field NMR needed to be cooled to near absolute zero, which defeated the purpose of removing the applied field in the first place. Instead, the researchers modified a different type of detector called an "optical atomic magnetometer" – which requires no refrigeration – for use at zero-field.

The team demonstrated its technique by distinguishing between several similar hydrocarbon



molecules – the first time that zero-field NMR has been successfully used for such complex chemical analysis.

Bernhard Blümich, an NMR spectroscopist at Aachen Technical University in Germany, is impressed. "This is a milestone paper," he says, "All these components you need are not very expensive or can be made inexpensive in the future. You come up with an NMR

spectrometer which is much less expensive than today's high-field spectrometers."

The research is published in *Nature Physics*.

### About the author

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### 8 comments

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### P-hydrogen