**////Title: Exploring the Potential of Metatorbernite in Uranium Remediation**

**////Standfirst:**

Although nuclear power is a clean alternative to fossil fuel combustion, this industry often causes uranium pollution in the local environment. The generation of metatorbernite, a solid material containing uranium, is one promising way to remove dissolved uranium atoms from industrial wastewater. However, before this remediation technology can be widely applied, we need a deeper understanding of the properties of metatorbernite, such as its long-term stability, to ensure that uranium will not be re-released from its structure. Dr Caroline Kirk, Ms Fi MacIver-Jones and their colleagues at the University of Edinburgh have been working to establish the structure and stability of this material, so that it can be applied for uranium remediation in the near future.

**////Main text:**

Since its discovery, uranium has proven to be an incredibly useful resource. Its use in generating nuclear power has solidified its necessity for the future. Unlike energy derived from fossil fuels, nuclear power doesn’t generate greenhouse gases – the primary culprit behind global climate change.

However, the use of uranium in nuclear power comes with several drawbacks. From mining to power generation, industries that process uranium incur the risk of contaminating the local environment. Because of its radioactive properties, uranium pollution has potentially devastating consequences, and can persist in the environment for a long time. As such, many scientists are attempting to develop methods that remediate uranium from the wastewater produced by nuclear power plants, and industries that mine and process uranium.

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One particularly interesting group of materials used in uranium remediation is called the ‘autunites’. These solid materials, which contain uranium, can be generated within wastewater streams, locking uranium atoms into their structures. Metatorbernite is a particularly promising autunite material, which contains copper alongside uranium. Because copper is often found in uranium ores, and thus in wastewater from uranium-based industries, metatorbernite may be generated within such waste streams, removing dissolved uranium and copper simultaneously from the water as the material forms.

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Compared to other autunites, metatorbernite is highly stable. However, there are still some uncertainties regarding the structure of the material, and how its structural properties are related to its stability. This makes it difficult to predict exactly how the material will behave under different industrial conditions. For instance, if metatorbernite were less stable under certain conditions, then it could break down and re-release uranium back into the waste stream, contaminating the environment.

Therefore, in order to use this material for large-scale remediation projects, we need a deeper understanding of its structural properties.

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Towards this aim, Dr Caroline Kirk, Fi MacIver-Jones and their colleagues at the University of Edinburgh have been working hard to gather data that could help to definitively establish the full structure of metatorbernite. In particular, the researchers wanted to determine the locations of certain hydrogen atoms, which form the water molecules inside the structure of metatorbernite.

This is important, because water molecules inside the material play a large role in holding the whole structure together. By locating the hydrogen atoms of these water molecules, we can determine the orientation of the molecules. This, in turn, can help scientists to learn more about the stability of metatorbernite under different conditions. However, previous research used techniques that struggled to locate these hydrogen atoms, mainly due to the dominance of the much larger uranium atoms, which overshadowed the hydrogen atom locations.

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Dr Kirk, Ms MacIver-Jones and their team set out to determine the locations of these atoms, by first synthesising their own samples of metatorbernite.

The team then gathered data on the structure of their metatorbernite samples using various analytical methods, the main one being a process called neutron powder diffraction. In this process, neutrons are fired into the sample at various angles. When these neutrons come into contact with atomic nuclei within the sample, they are scattered in various directions. These scattered neutrons can then be measured by a detector. The pattern of scattered neutrons can be analysed to provide a good indication of which atoms are located where within the structure of a material.

Neutron powder diffraction analysis is highly specialised, and can provide important and complementary information to more common techniques, such as X-ray powder diffraction. There are only a few facilities around the world that can carry out this type of research, including the UK’s Neutron and Muon Facility, where Dr Kirk’s team analysed their metatorbernite samples. Therefore, it was imperative that the team gathered as much data from this process as they could.

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Through the use of neutron powder diffraction, the team was able to gather new data that revealed the positions and orientations of water molecules within the structure of metatorbernite. In addition, by analysing the data that they gathered, the researchers were able to figure out how these water molecules are able to interact with one another, providing the bonds that hold the material together to form a stable structure.

This information is absolutely crucial when it comes to understanding the stability and physical properties of metatorbernite. From this, scientists will be able to much determine whether the generation of this material within wastewater streams is a suitable method of uranium remediation.

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Through the innovative use of an incredible analytical technique, Dr Kirk, Ms MacIver-Jones and their team have collected critical data that has allowed them to determine the detailed structure of metatorbernite. From this work, the scientific community now has a much better understanding of the properties of this material, including its stability. The team’s work paves the way for future research, to further determine how metatorbernite can be best used to remediate uranium, helping industries to protect the natural environment.

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This SciPod is a summary of the paper ‘Locating hydrogen positions in the autunite mineral metatorbernite [Cu(UO2)2(PO4)28H2O]: a combined approach using neutron powder diffraction and computational modelling’ from the *International Union of Crystallography Journal,* [doi.org/10.1107/S205225252100837X](https://doi.org/10.1107/S205225252100837X).