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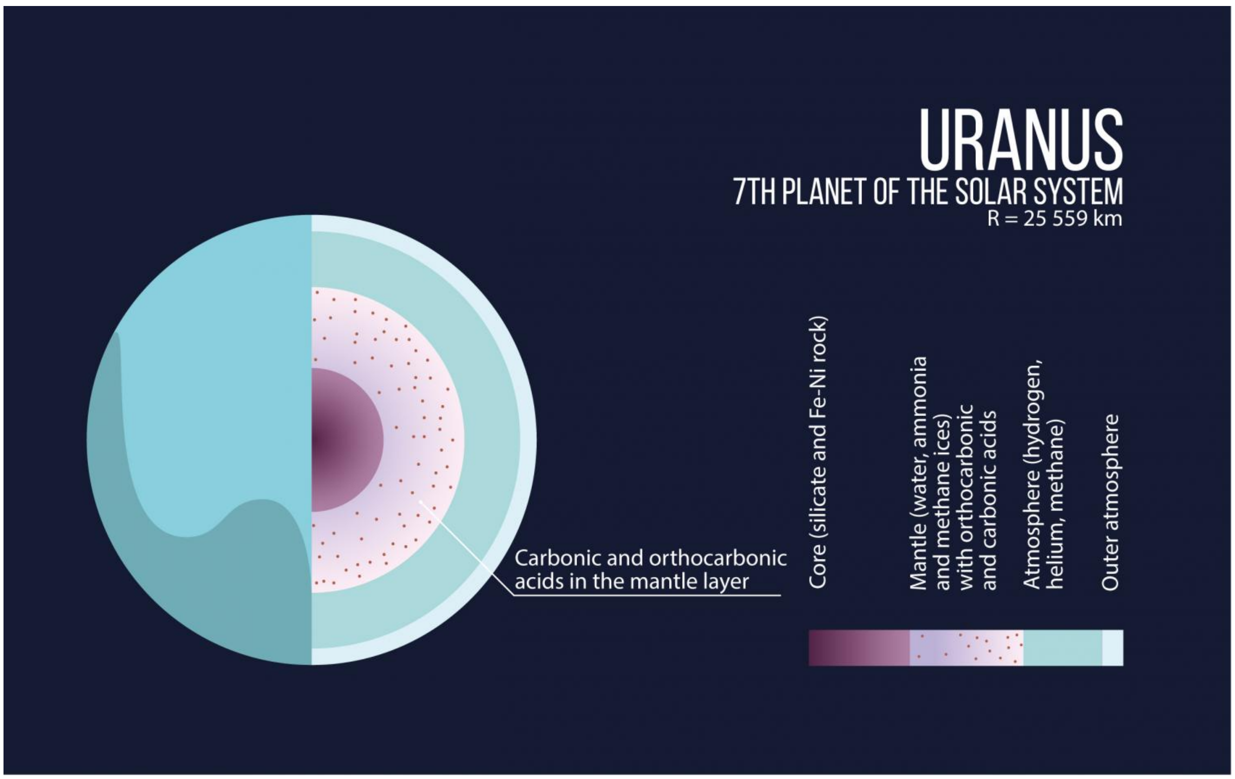
# Scientists discover extraordinary compounds that may be hidden inside Jupiter and Neptune

September 6 2016



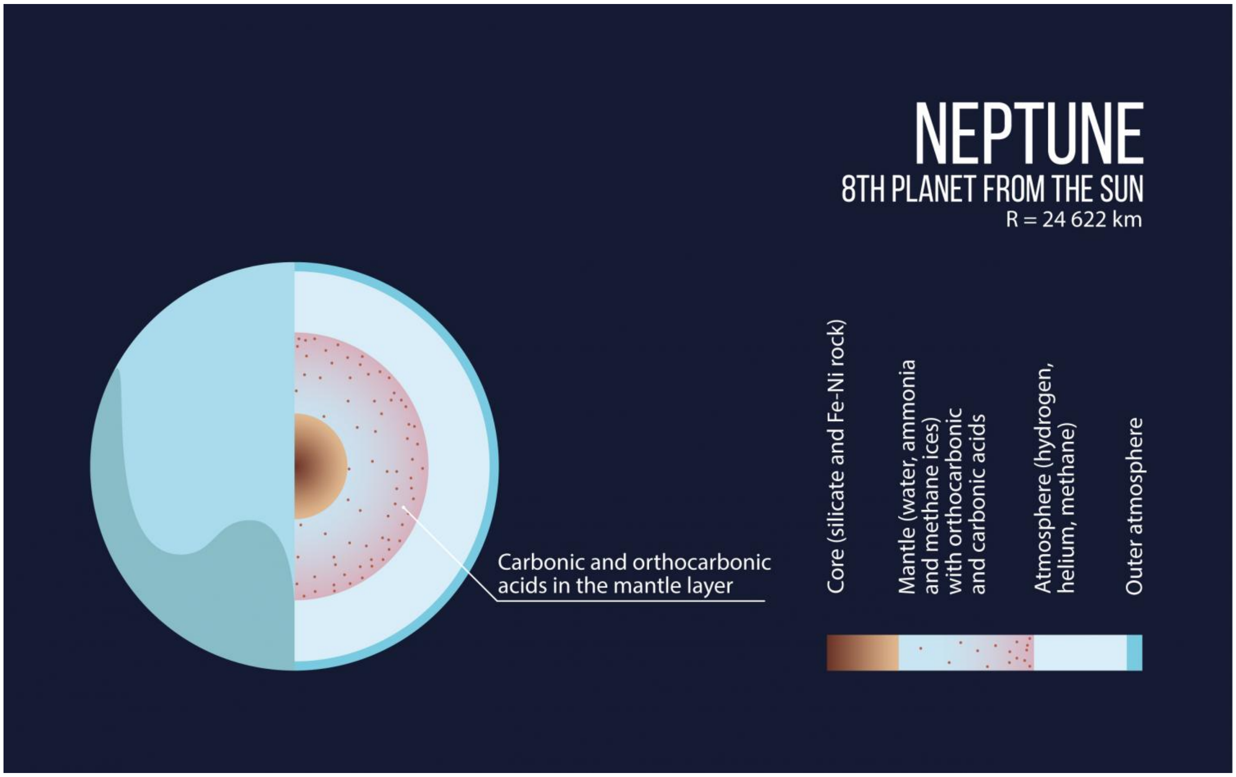

The interior structure of Uranus. Credit: Moscow Institute of Physics and Technology

Using computer modeling, Russian researchers have described what molecules may be present in the interiors of Uranus, Neptune, and the icy satellites of the giant planets. The scientists discovered that at high pressures, which are typical for the interiors of such planets, exotic molecular and polymeric compounds are formed. These compounds include carbonic acid and orthocarbonic acid. The results of the study have been published in the prestigious journal *Scientific Reports*.

"The smaller gas giants – Uranus and Neptune – consist largely of carbon, hydrogen and oxygen. We have found that at a pressure of several million atmospheres unexpected compounds should form in their interiors. The cores of these planets may largely consist of these exotic materials," says the study's lead author Artem Oganov, professor of Skoltech and the head of MIPT's Computational Materials Discovery Lab.

A team led by Professor Oganov developed the world's most universal and powerful algorithm for crystal structure and compound prediction – USPEX (Universal Structure Predictor: Evolutionary Xtallography). In recent years, scientists have used this algorithm to discover several substances that are "forbidden" in classical chemistry and that may be stable at high pressures. These include a number of previously unknown variants of salt – $Na_3Cl$, $NaCl_3$, $NaCl_7$ and even $Na_3Cl_2$ and$Na_4Cl_3$, as well as exotic new oxides of magnesium, silicon and aluminium that may exist in the interiors of super-Earths.

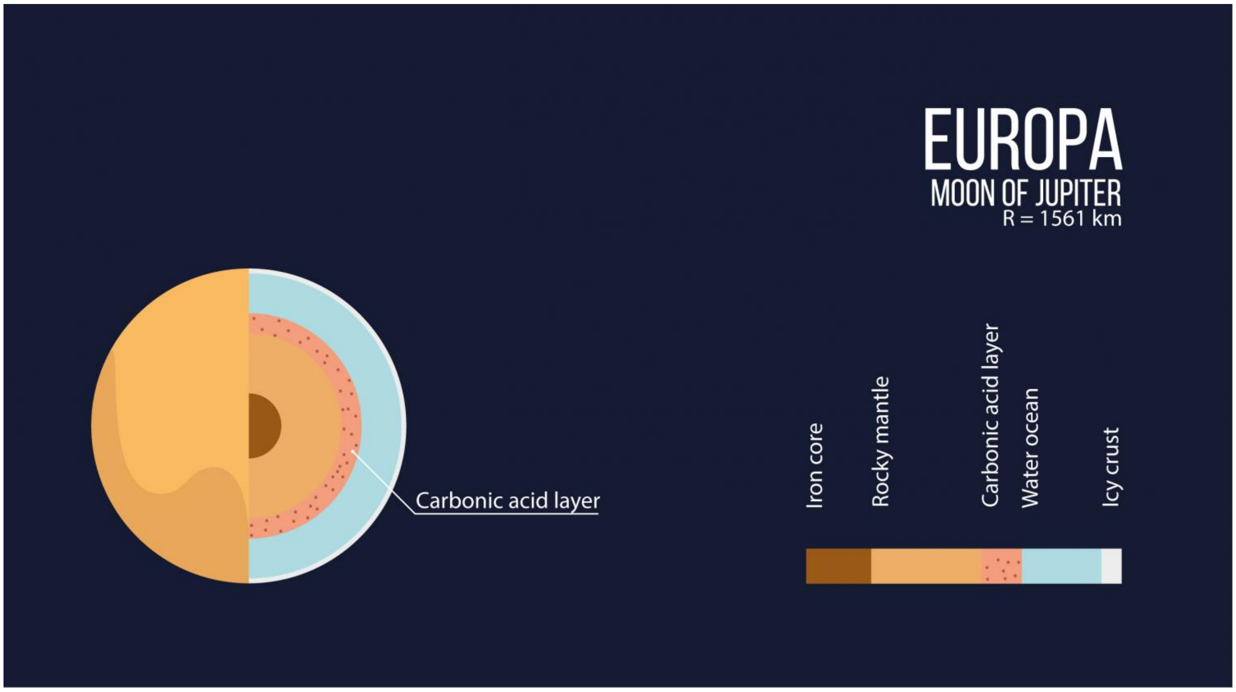
Now Oganov and his co-author Gabriele Saleh from MIPT have decided to study the chemical behaviour of the carbon-hydrogen-oxygen system under high pressure. "This is an extremely important system, because all organic chemistry 'rests on' these three elements, and until now it had not been entirely clear how they behave under extreme pressures and temperatures. In addition, they play an essential role in the chemistry of the giant planets," says Oganov.




The interior structure of Neptune. Credit: Moscow Institute of Physics and Technology

The scientists knew that under atmospheric pressure, all compounds of carbon, hydrogen and oxygen, except for methane, water, and carbon dioxide, are thermodynamically unstable. With an increase in pressure, water and carbon dioxide remain stable, but at pressures above 93 gigapascals (0.93 million atmospheres)methane begins to decompose, forming heavy hydrocarbons – ethane, butane, and polyethylene. At a lower pressure—approximately 4 GPa—methane and molecular hydrogen interact, forming co-crystals (where two molecules together create one crystal structure), and at 6 GPa, hydrates—CO-crystals made of methane and water—are formed. To put this into context, the pressure at the bottom of the Mariana Trench (the deepest part of the world's oceans) is 108.6 megapascals, which is one thousand times lower.

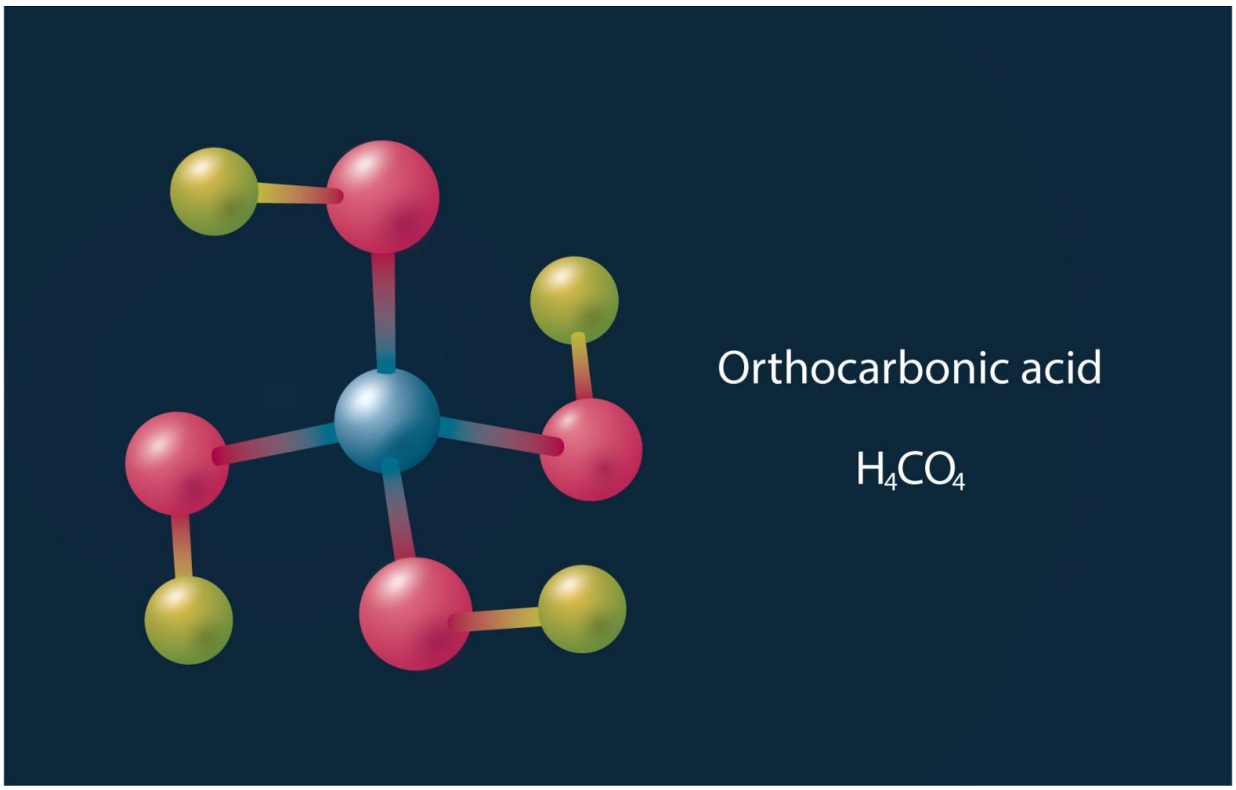
Oganov and Saleh took on the task of finding all stable compounds in the range up to 400 GPa (around 4 million atmospheres) and discovered several new substances. These included a clathrate (inclusion compound, a type of co-crystal) of molecular hydrogen and methane 2CH4:3H2, which is stable in the pressure range 10-215 GPa.




The interior structure of Jupiter's moon - Europa. Credit: Moscow Institute of Physics and Technology

The scientists also found that at a pressure above 0.95 GPa (approximately 10,000 atmospheres), carbonic acid (H2CO3) becomes thermodynamically stable. This is very unusual for a substance that is highly unstable under normal conditions – strong acids are needed for its synthesis and it can only exist in a vacuum at very low temperatures, the authors write.

"It is possible that the cores of Neptune and Uranus may contain significant amounts of a polymer of carbonic acid and orthocarbonic acid," says Oganov.




Orthocarbonic acid (also known as Hitler's acid). Credit: Moscow Institute of Physics and Technology

**More information:** Gabriele Saleh et al. Novel Stable Compounds in the C-H-O Ternary System at High Pressure, *Scientific Reports* (2016).

DOI: 10.1038/srep32486

Provided by Moscow Institute of Physics and Technology