

Visual depiction of the energetic nitroamine molecule CL-20. ([Download Image](#))

Study on stability of highly energetic materials

Anne M Stark, stark8@llnl.gov, 925-422-9799

Understanding the physical and chemical characteristics of energetic materials under extreme conditions is crucial for their safe and efficient use. High-pressure phase transitions in such materials can cause significant changes in their initiation properties and detonation performance necessitating detailed structural studies.

The high-pressure structural evolution of CL-20 is of particular interest due to its high energy density content, which opens it to be an important material in future applications. However, previous experimental work only determined the equation of state up to approximately 7 GPa (70,000 atmospheres of pressure).

Researchers from LLNL have investigated the ambient-temperature high-pressure phase stability of ϵ -CL-20 — the most stable and highest density polymorph, to pressures five times as high as previously done using synchrotron powder X-ray diffraction.

Lead author of the research, Samantha Clarke, explains “by using the high flux available at modern synchrotron sources, we are able to probe ϵ -CL-20 to much higher pressures and find that the ambient phase remains stable upon compression to the highest pressure reached.”

The diffraction experiments were performed at the HPCAT beamline at the [Advanced Photon Source](#), Argonne National Laboratory. The research appears in *JANNAF Journal of Propulsion and Energetics*.

An intriguing finding of the project was that the compressibility of each of the axes is similar over the entire pressure range, unlike many other energetic compounds; this was attributed to the cage-like structure of the molecule. The team determined experimental equation of state parameters from the diffraction data, which match extremely well with the calculated values. Group leader Richard Gee led density functional theory calculations and said: “The excellent agreement between the experimental and modelled data highlights the strength of such combined efforts.”

The results of this study enable more accurate safety and performance modeling of this material and its formulations. Clarke and Gee were joined on the publication by I-Feng Kuo, Joseph Zaug, Sorin Bastea, Ana Racoveanu, Keith Coffee and Elissaios Stavrou.

Tags: [Physical & Life Sciences](#)

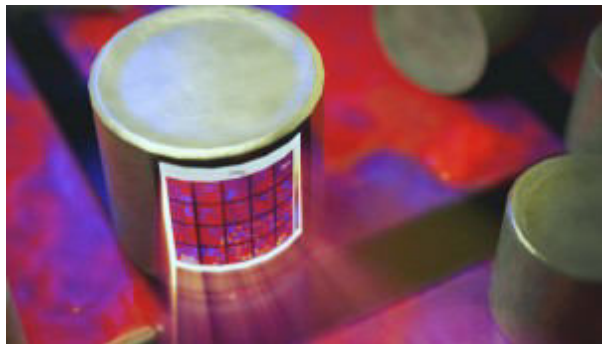
RELATED LINKS

[Advance Photon Source](#)

FEATURED ARTICLES



World's largest optical lens shipped to SLAC



Going small can help determine where nuclear material came from and how it was made



Freshening up contaminated water

EL CAPITAN CLIMBS THE LADDER



See what 'The Next Platform' says

LLNL.GOV

Missions

Science & Technology

Programs

Doing Business

News

About

Careers

Community

PROGRAMS

Weapons

Global Security

Lasers

Physical and Life Sciences

Engineering

Computing

RESOURCES

Contact

Visiting

Emergency Communication

Research Ethics

Privacy

Copyright and Reuse

Site Map

STAY CONNECTED



[↑ Back to top](#)



Lawrence Livermore National Laboratory 7000 East Avenue • Livermore, CA 94550

Operated by Lawrence Livermore National Security, LLC, for the Department of Energy's National Nuclear Security Administration.



LLNL-WEB-458451 | [Privacy & Legal Notice](#)