Researchers design rare-earth extractants with the help of new software

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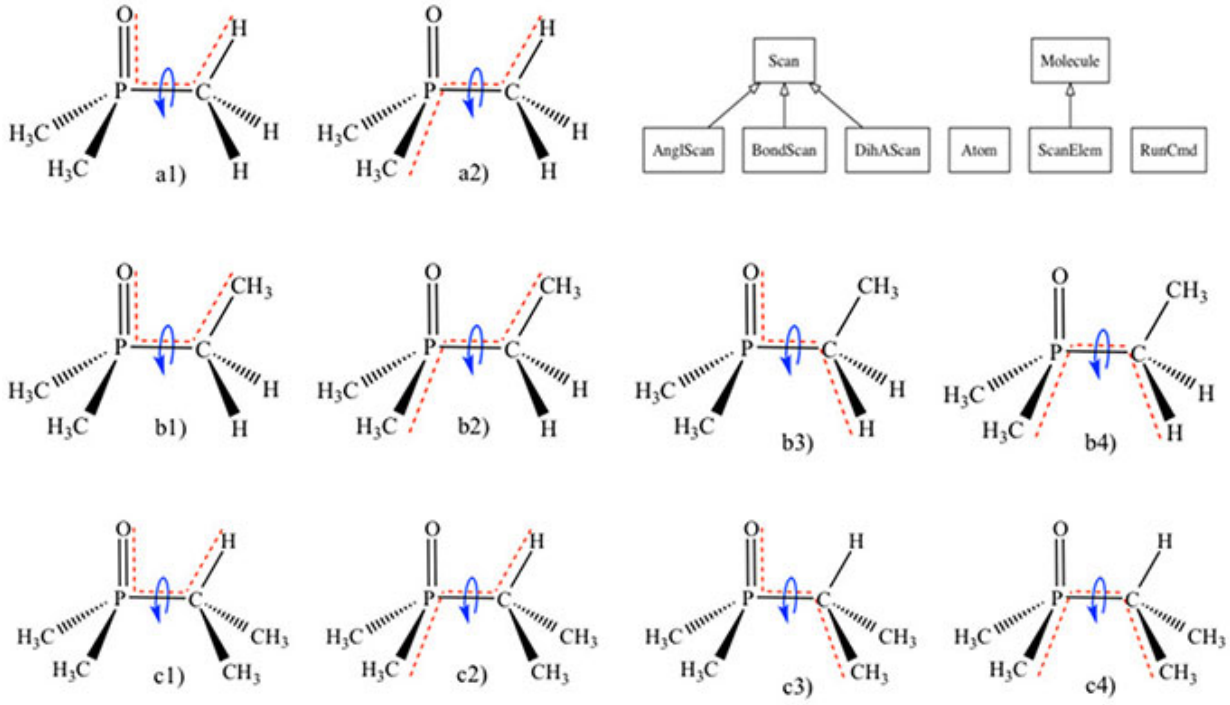

Credit: Ames Laboratory

The U.S. Department of Energy's Critical Materials Institute has developed a computer program, called ParFit, that can vastly reduce the amount of time spent identifying promising chemical compounds used in rare-earth processing methods.

Testing and developing more efficient and environmentally friendly ways of extracting rare-earth metals as speedily as possible is a primary goal of CMI. Rare-earth metals are vital to many modern energy technologies, but high commercial demand and mining challenges have made optimizing our country's production and use of them of vital importance.

"Traditional, quantum mechanical methods of predicting the molecular design and behavior of these extractants are too computationally expensive, and take too long for the timescale needed," said software designer and CMI scientist Federico Zahariev. "So we developed a program that could create a simpler classical mechanical model which would still reflect the accuracy of the quantum mechanical model."

ParFit uses traditional and advanced methods to train the classical mechanical model to fit quantum mechanical information from a training set. These classical models can then be used to predict the shape of new extractants and how they bind to metals.

"Roughly speaking, think of the molecule's shape and structure as a system of springs, where there might need to be a lot of small tightening or loosening of different connections to make it work correctly," said CMI Scientist Theresa Windus. "It's the same way in which we apply the quantum mechanical calculations to create these classical mechanical models—it's a tedious, error-prone, and lengthy process. ParFit makes this as quick as possible, automates the fitting of those parameters, and accurately reproduces the quantum mechanical energies."

"The program's capabilities enable the researchers to model an almost unlimited number of new extractants," said software developer and CMI Scientist Marilu Dick-Perez. For example, the classical models used in the software code, HostDesigner – developed by Benjamin Hay of Supramolecular Design Institute, creates and quickly assesses possible

extractants for viability and targets extractants that are best suited for further research. "We've reduced the computational work from 2-3 years down to three months," she said. "We've incorporated as much expert knowledge into this program as possible, so that even a novice user can navigate the program."

The software's capabilities is further discussed in a paper, "ParFit: A Python-Based Object –Oriented Program for Fitting Molecular Mechanics Parameters to ab Initio Data", authored by Federico Zahariev, Nuwan De Silva, Mark S. Gordon, Theresa L. Windus, and Marilu Dick-Perez, and published in the *Journal of Chemical Information and Modeling*.

More information: Federico Zahariev et al. ParFit: A Python-Based Object-Oriented Program for Fitting Molecular Mechanics Parameters to ab Initio Data, *Journal of Chemical Information and Modeling* (2017). DOI: 10.1021/acs.jcim.6b00654

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