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# Spectroscopic Signature of Noncovalent Bonds

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## Recommended Citation

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Data Management Plan

1. The primary outcome of the proposed research will be data extracted from computational calculations of the target chemical systems. The output data will be stored in the form of .log files for greatest ease of storage and transferability, typically 2 MB each. It is anticipated that each subproject will generate on the order of 50-100 such files. A course will be taught for advanced undergraduate and graduate students which provide instruction and hands-on participation in computational methods in chemistry and biochemistry. A syllabus will be prepared for this course, as well as instructional material and class notes.

2. Standards applied to the data will be the standard methods of the field. Quantum methods will be of state-of-the-art quality, incorporating electron correlation and large basis sets. These files will contain not only the atomic coordinates, but also the wave functions that can be analyzed by others. Data will be stored in standard log files, as well as pdf in some cases.

3. Data will be analyzed, and the results submitted for publication in peer-reviewed journals. Journals envisioned at this time include J. Am. Chem. Soc., J. Phys. Chem. Phys Chem Chem Phys, Chem Phys, Chem Phys Lett, ChemPhysChem, and Chem Eur. J. Summaries of the data will also be disseminated via presentations at scientific meetings, both national and international. The geometries and primary extracted data will be placed on the group's website prior to publication. In addition, much of this information will also be added to the Supporting Information sections maintained by the journals in which they are published. The syllabus and class material for the computational chemistry course will be available via the internet to all interested parties. Another repository for all data generated, including syllabus and course materials, will be the DigitalCommons@USU website. All of these data will be available to interested parties without the need to request permission.
Results of Research will be made available to the public in several ways:

- Prior to publications the geometries and primary extracted data will be placed on the group's website.
- Data supporting journal publications will be added to the Supporting Information sections maintained by the journal, when available.
- Journal articles will be deposited in NSF's Public Access Archive.
- Data, syllabus, and course materials will be archived in DigitalCommons@USU, USU's institutional repository. All files archived here are backed up at multiple sites, including cloud storage. Preservation copies are stored in Amazon Web Services, with redundant storage across multiple facilities and are regularly verified for integrity of data using checksums. DigitalCommons@USU's metadata is based on the Dublin Core metadata standard. Data files are accompanied by appropriate README and other documentation files to ensure future usability of data.

4. Data reported in the literature will be available for re-use and re-distribution according to copyright privileges of each journal where the work appears. The original information from which the publications are derived will be publicly available. Those requesting additional original data will have their requests honored by the research team. The most likely audience will be researchers in this area, as well as educators interested in developing a computational chemistry course.

5. The publications will be available in the public domain as per the policies of each journal where the work is published. The original data will be maintained on the computers of the research team for future access. This information will be stored for at least two years after termination of the project. The storage will be in several places, including group computers and servers, as well as the USU repository.