

The Chemical and Biochemical Reference Data Division from NIST

Partner contact person: Carlos Gonzalez

Where experimental, theoretical, and computational research is performed on the identity and reactivity of chemical species (including small molecules, aerosols, proteins, nanoparticles and biomolecules), emphasizing data, information and protocols for the identification of chemical and biochemical species; validation, implementation and innovation of computational chemistry tools and techniques; experimental, theoretical, and computational studies of the thermochemistry, kinetics and mechanisms of chemical reactions in the gas and liquid phases and at interfaces; develops. Our contact, Dr. Carlos Gonzalez is a quantum chemist by training and the Chief of the Division in charge of overseeing the design, implementation and validation of all data products within the Division, including NIST Chemistry WebBook (one of NIST's most popular data product), the NIST-EPA Mass Spectrometry Data Library, the Computational Chemistry Comparison and Benchmark Database, and NIST Chemical Kinetics Database. The inclusion of this external partner is of primary importance for the study of interoperability with other A+M schemes, involving fields on the scale of A+M data, i.e. chemistry and biology.

[Back to Partners](#)