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Reaction Roulette: Utilizing *Elemental* MS/MS for the Characterization of Gas Phase Ion-Molecule Interactions

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Tandem mass spectrometry (MS/MS) is a fairly recent addition to the analytical chemist toolkit for *elemental* analysis. Elemental MS/MS instruments have two mass filters with a collision/reaction cell (CRC) in between that can be used to effect desirable ion-molecule reactions. The key analytical advantage of this feature is that it allows for the in-line separation of analytes from isobaric interferences which would otherwise require lengthy off-line and sometimes complicated sample preparations, like ion exchange chemistry. It also enables in situ separations in cases where bench chemical separations are not possible, e.g., in laser ablation sampling. Instrumentation capable of elemental MS/MS have only been commercially available since 2012. In this talk, we will discuss our work in exploring the reactivity of 45 elements spanning almost all groups of the periodic table with N_2O and CO_2 using the Agilent 8900 QQQ-ICP-MS. Reasonable correlations between independent Density Functional Theory (DFT) derived reaction enthalpies, calculated using NWChem, and the reaction data were found, showing that reactions typically proceed when thermodynamically allowed. Our work demonstrates the utility of two relatively new platforms (commercial elemental ICP-MS/MS and EMSL Arrows interface to the NWChem program suite developed at the Environmental Molecular Science Laboratory (EMSL) at the Pacific Northwest National Lab (PNNL)) for the study of a large number of elements simultaneously and within a very short period of time. The ease and rapidity of data collection and DFT calculations has potential to revolutionize the identification of targeted reaction chemistries to be leveraged for analytical method development, such as for the in-line separation of isobaric interferences from analytes of interest.