THE STRUCTURE OF ISOLATED $TeSe$ FROM ROTATIONAL INVESTIGATIONS: BOND LENGTHS, ROTATIONAL PARAMETERS, AND HYPERFINE CONSTANT

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Laser ablated tellurium selenide clusters were isolated in pulsed rare gas supersonic expansions. With the production conditions monitored and optimized by the aid of time-of-flight (TOF) mass spectrometry, surprisingly strong pure rotational transitions originating from low-J energy levels were found in a search guided by high level Coupled Cluster calculations.

As the first intermetallic group VI compound investigated microwave spectroscopically we were able to identify the electronic ground state rotational spectra of 43 isotopomers of the tellurium selenide dimer in natural abundance by Fourier transform microwave (FT-MW) spectroscopy. The recorded rotational transitions from $J' - J = 1 - 0$ up to $J' - J = 7 - 6$ cover a frequency range from 3.6 to 26.4 GHz. Furthermore, the microwave spectra of the first six vibrationally excited states of the three most abundant isotopomers were observed.

The dataset can be analysed using a multi-isotopomer fit to a Dunham-type expression which includes terms that allow for Born-Oppenheimer breakdown corrections. The transitions of 16 isotopomers, either containing ^{125}Te or ^{123}Te and/or ^{77}Se showed splittings due to spin-rotation coupling. The rotational parameters and spin-rotation constants for those species in their vibrational ground state were obtained by fits processed for each isotopomer separately.