EXHAUSTIVE PRODUCT ANALYSIS OF THREE BENZENE DISCHARGES BY MICROWAVE SPECTROSCOPY

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By means of chirped and cavity microwave spectroscopies, automated double resonance, new high-speed fitting and deep learning algorithms, and large databases of computed structures, the discharge products of three benzene mixtures – alone or with oxygen and nitrogen – have been exhaustively characterized between 6.5 and 26 GHz. In total, more than 3300 spectral features were observed; 88% of these, accounting for roughly 97% of the total intensity, have now been assigned to 160 distinct chemical species and 60 of their variants (i.e. isotopic species and vibrationally excited states). Roughly 50 of the products are entirely new or poorly characterized at high resolution, including many heavier than the precursor benzene. These findings provide evidence for a rich architecture of two- and three-dimensional carbon, and indicate that benzene growth, particularly formation of ring-chain molecules, occurs facilely under our experimental conditions. The present analysis vividly demonstrates the utility of microwave spectroscopy as a precision tool for complex mixture analysis, irrespective of whether the rotational spectrum of a product species is known a priori or not. From this large quantity of data, for example, it is possible to derive a mass spectrum for each discharge that is analogous to a traditional mass spectrum, but with exquisite isomeric resolution.