HIGH-RESOLUTION INFRARED SPECTROSCOPY OF CARBON-SELENIUM CHAINS: SeC₃Se and C₃Se

THOMAS SALOMON, I. Physikalisches Institut, Universität zu Köln, Köln, Germany; YURY CHERNYAK, JOHN B DUDEK, Department of Chemistry, Hartwick College, Oneonta, NY, USA; JÜRGEN GAUSS, Institut für Physikalische Chemie, Universität Mainz, Mainz, Germany; STEPHAN SCHLEMMER, SVEN THORWIRTH, I. Physikalisches Institut, Universität zu Köln, Köln, Germany.

To date, carbon-selenium clusters have received little attention from both experiment and quantum-chemistry. Recent high-resolution infrared survey scans of the ablation products from carbon-selenium targets in the 5μ m regime have revealed two bands previously not observed in the gas phase. On the basis of comparison with high-level quantum-chemical calculations performed at the CCSD(T) level of theory these bands are attributed to the linear SeC₃Se and C₃Se chains. Following the microwave detection of diatomic CSe some 45 years ago^a the present work marks the first high-resolution detection of polycarbon selenium clusters.

^aJ. McGurk, H. L. Tigelaar, S. L. Rock, C. L. Norris, and W. H. Flygare, J. Chem. Phys. 58, 1420 (1973).