

Abstract Submitted  
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**Highly Excited States of Chlorine Substituted Polyatomic Molecules in the Vacuum-Ultraviolet**<sup>1</sup> QUYNH NGUYEN, JILA Department of Physics and Chemistry, University of Colorado Boulder, WILLIAM PETERS, JILA Department of Physics, University of Colorado Boulder, RYAN FORTENBERRY, Department of Chemistry and Biochemistry, Georgia Southern University, MARGARET MURNANE, HENRY KAPTEYN, JILA Department of Physics, University of Colorado Boulder — Electronic states up to the vacuum-UV range and ionization potentials of the chlorine-substituted cumuleneone series are computed with the coupled cluster methods in order to explore the valence and Rydberg properties of lone-pair terminated,  $\pi$ -conjugated systems in potential resonance with lone pairs from elsewhere in the system. The carbon chain elongation within the family, ClHC<sub>n</sub>O, influences the electronic excitations, characters, and ionization potentials. Comparison between the hydrocarbons and the corresponding chlorinated derivatives give notable similarities. An increase of Rydberg mixing with valence character is observed, which causes these highly energetic states to be more diffuse and hence, more challenging to study. Thus, we explore the effects of diffuse basis functions to accurately predict the photophysical properties of the systems. Future implications for sub-fs ultrafast dynamics in highly excited states of polyatomic molecules will be discussed.

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