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Nota di contenuto	Previous Experimental and Theoretical Results for l-C3H+ and C4 -- Theoretical Methods -- Results for l-C3H+ -- Results for C4 in its X3g-Ground State.
Sommario/riassunto	In this thesis accurate predictions for the spectroscopic parameters of l-C3H+ and C4 are made from state-of-the-art electronic structure calculations. Both molecules are of interest to interstellar cloud chemistry and only scarce experimental information about their rovibrational properties is available. Christopher J. Stein recapitulates the basics of the computational methods applied and gives an in-depth description of the computer program developed for the rovibrational calculations. Contents Previous Experimental and Theoretical Results for l-C3H+ and C4 Theoretical Methods Results for l-C3H+ Results for C4 in its X3g-Ground State Target Groups Lecturers and Students of Theoretical Chemistry, Spectroscopy and Astrochemistry The Author Christopher J. Stein is currently pursuing his PhD degree at the Theoretical Chemistry group of Prof. Dr. Markus Reiher at ETH Zurich. His research is focused on the development of new wave function

methods and the automation of quantum-chemical multi-reference calculations.