

Part II

Introduction

The starting point for this work was the dataset obtained during the optical longterm-monitoring program of comet C/1995 O1 Hale-Bopp [Rauer *et al.*, 1997, 2002]. Observations started in April 1996 and ended nearly 5 years later in January 2001 covering a heliocentric distance range from 4.6-2.8 AU pre-perihelion and from 2.9-12.8 AU post-perihelion. It was the longest campaign ever observing a single comet in the optical wavelengths range so far. This huge dataset had to be reduced and analyzed. During a first analysis using the Haser model a number of scientifically interesting questions arose, which had to be analyzed further in more detailed studies. One of these was especially interesting: the formation of C₂ and C₃ in a cometary coma.

C₂ has been the first constituent of the coma to be found by spectroscopy observations. This was done already in 1864 by Giovanni Donati [1864] in comet Tempel (1864 II) and independently in 1867 by Sir William Huggins [1867] in comet Winnecke (1867 II). Both identified the emissions by comparing the cometary spectra with flame spectra. They also observed a group of lines near 4050 Å, but it took more than eighty years until Douglas [1951] identified these lines as C₃ emissions. For more than a century C₂ remained without an observed parent molecule. A number of parent molecules had been proposed, namely acetylene C₂H₂ and ethane C₂H₆ for C₂ [Jackson, 1976] and propyne or its isomeric form allene C₃H₄ for C₃ [Stief *et al.*, 1972]. Finally in 1996 emissions of C₂H₂ and C₂H₆ have been detected in comets Hyakutake and Hale-Bopp [Tokunaga *et al.*, 1996; Brooke *et al.*, 1996; Mumma *et al.*, 1996]. C₃ is up to the present without an observed parent molecule.

The main aim of this study is to analyse the formation of C₂ and C₃ in a cometary coma at large heliocentric distances. As Crovisier and Encrenaz [2000] pointed out in their book on comets: C₂ has been an orphan for nearly a century. To stay in this picture, this work will help to link the 'orphan' with its heritage by providing a family tree and will attempt to identify the ancestor of C₃. In this work a chemical reaction network is presented capable of explaining the formation of C₂ and C₃ assuming C₂H₂, C₂H₆ and C₃H₄ as their parent molecules. Such a formation model allows to derive abundances for these parent molecules from data obtained with optical spectroscopy at heliocentric distances $r_h \geq 3$ AU. Up to now C₂H₂ and C₂H₆ has only been measured by infrared observations at heliocentric distance $r_h \leq 3$ AU [Dello Russo *et al.*, 2001]. Thus this model can greatly extend the heliocentric distance range over which hydrocarbons can be studied in the coma of comet Hale-Bopp. Based on the production rates for C₂H₂, C₂H₆ and C₃H₄ abundances ratios will be derived for heliocentric distances $r_h \geq 3$ AU. Especially the ratio to CO at these large heliocentric distances can give some important indications on the volatility of the C₂ and C₃ parent molecules.

This work consists of three main parts. The first part is an introduction to the areas of cometary science touched in this study. Its intention is to give a short introduction in each topic. A more detailed discussion is given only for issues closely related to this study. The second part presents the dataset obtained during the optical longterm monitoring program of comet Hale-Bopp [Rauer *et al.*, 1997, 2002], describes the data reduction and presents a first analysis using the Haser model. The third part finally presents the analysis of the formation of C₂ and C₃ and the derived formation model. Using this model abundances for C₂H₂, C₂H₆ and C₃H₄ at heliocentric distances greater than 2.86 AU have been derived.

This part is closed by a discussion on the implications for the formation region of comet Hale-Bopp.