Formation of c-SiC_3 molecules in the circumstellar envelope of AGB stars

A recent study led by Dr. Yang Tao (杨涛) from the State Key Laboratory of Precision Spectroscopy in the East China Normal University, Dr. Ralf Kaiser from the University of Hawaii at Manoa and Dr. Martin Head-Gordon from the University of California at Berkeley unveiled the mysterious reaction mechanism involving silicon-bearing molecules such as c-SiC_3 in the circumstellar envelope of carbon stars, which has been published in *PNAS* (2019, 116: 14471—14478), under the support of the National Natural Science Foundation of China, the Fundamental Research Funds for the Central Universities and so forth.

For decades, the carbon-rich asymptotic giant branch (AGB) star IRC+10216 (CW Leo) has been widely recognized as a rich, natural laboratory for advancing our fundamental understanding of the chemical evolution of the carbon-rich circumstellar envelopes through astronomical observations combined with astrochemical modeling exploiting complex gas phase reaction networks. Although complex organosilicon molecules are ubiquitous in the circumstellar envelope of IRC+10216, their formation mechanisms have remained largely elusive until now.

Exploiting silicon tricarbide (c-SiC_3) as a benchmark, they provide evidence from laboratory experiments, electronic structure calculations, and astrochemical modeling that, organosilicon species can be synthesized via distinct chemistries in the inner and outer envelope of carbon stars like IRC+10216 via bimolecular reactions followed by photochemical dehydrogenation to bare silicon carbon molecules. This system illustrates the concept of an excited-state-induced synthesis of exotic organosilicon molecules (SiC_3H_2) in the inner circumstellar envelope via the reaction of electronically excited silicon atoms with ubiquitous hydrocarbons, with the parent species undergoing photochemical processing in the outer envelope to cyclic silicon tricarbide (c-SiC_3). These mechanisms are of fundamental significance to facilitate an understanding of how carbon and silicon chemistries can be coupled to synthesize organosilicon molecules in the universe.

A rapid development of the telescopes of high sensitivity and resolution has been well promoted in the most recent years, such as the 500-m Aperture Spherical Telescope in Guizhou (FAST), Tianma 65-m Aperture Radio *Telescope in Shanghai*, Steerable 110-m Aperture Radio Telescope *from Xinjiang Observatory and so forth. The finding above can therefore facilitate the* interdisciplinary interaction of the physical chemistry experiments and computations as well as the astronomical observation, paving the way to understand how the universe evolves in the chemical manner.

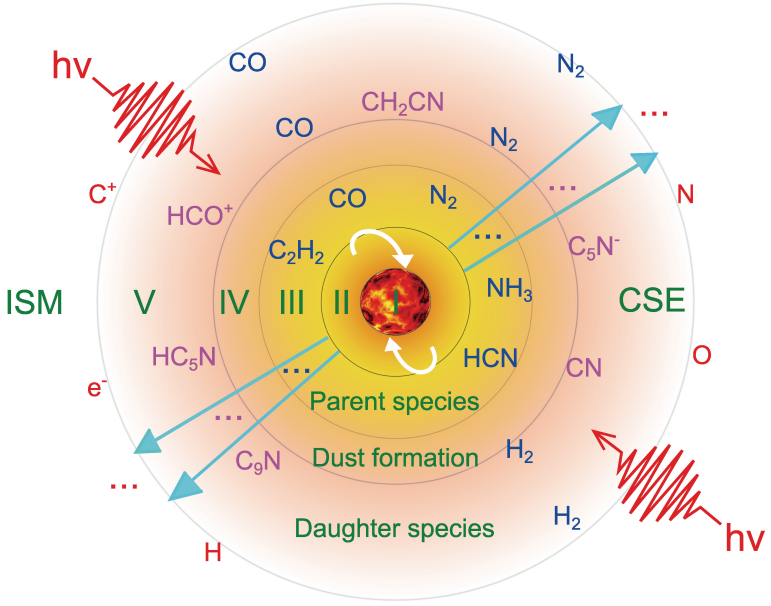

Figure Illustration of molecular distribution in the circumstellar envelope of IRC+10216.