View metadata, citation and similar papers at core.ac.uk
brought to you by CORE
provided by Illinois Digital Environment for Access to Learning and Scholarship Repository

TOWARDS A MECHANISM FOR FORMATION OF SILICON CARBIDE CRYSTALS IN AGB STARS

JESSE J LUTZ, *Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, OH, USA*; XIAOFENG F DUAN, *DoD Supercomputer Resource Center, Air Force Research Laboratory, Wright-Patterson AFB, OH, USA*; LARRY W BURGGRAF, *Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, OH, USA*.

Silicon carbide (SiC) grains comprise a significant fraction of the dust found around carbon-rich AGB stars. Their presence in the interstellar medium is thought to originate from self-assembly of organosilicon building blocks, including previously observed species such as carborundum and cyclic silicon dicarbide (c-SiC_2). However, the actual formation mechanisms of even these simple silicon-bearing organic molecules remains elusive. Here it is proposed that disilyne (Si_2H_2) reacts barrierlessly with abundant acetylene (C_2H_2) on a spin-conserving potential to form $C_2Si_2H_4$. This species has been shown in experimental and theoretical studies[a] to photoisomerize under UV irradiation resulting in the formation of several species, one being a c-SiC_2 precursor and another being a highly polar species capable of supporting a dipole-bound electron. This strongly dipolar $C_2Si_2H_4$ isomer may represent the missing link supporting the molecular aggregation hypothesis for SiC formation. Importantly, its polarity drives molecular aggregation, and, after subsequent oxidation to C_2Si_2, its heteronuclear linkages are well-prepared for SiC nucleation, presumably initiated by a shock-wave pulsation event. Past theoretical studies by our group[b,c] are combined with new results, computed at the DFT and coupled-cluster levels of theory, to support the proposed mechanism.

[a] Lutz J.J., Inorganics, *submitted*

[b] Lutz J.J., Duan X.F., et al. J. Chem. Phys. 148, 174309 (2018)

[c] Byrd J.N., Lutz J.J., et al. J. Chem. Phys. 145, 024312 (2016)