Formation of Sodium-bearing species in the interstellar medium

E. Herbst,[1] K. Acharyya,[2] and D. E. Woon[3]

[1]*Departments of Chemistry and Astronomy, University of Virginia, USA*
[2]*Planetary Sciences Division, Physical Research Laboratory, India*
[3]*Department of Chemistry, University of Illinois at Urbana-Champaign, USA*

Sodium-bearing species such as NaCl in the gas-phase have been observed in an assortment of stellar atmospheres and interstellar environments. [1],[2] However, their detection in relatively low-temperature regions has yet to be made. Here we emphasize NaCl via both gas-phase and grain-surface chemistry under assorted interstellar conditions. Two types of numerical gas-grain simulations have been run: models under isothermal conditions at temperatures from 10 K to 800 K with varied intervals, and three-phase warm-up models that consist of an initial isothermal collapse at 10 K, a warm-up phase, in which temperature reaches 200 K with varied intervals, and lastly a hot-core phase. The surfaces of dust grains contain water-ice using a base cluster of 17H2O. Desorption and barriers against diffusion were calculated with Gaussian 09 using B3LYP density functional theory. We found that for isothermal models over a broad parameter space, the fractional abundances of gaseous NaCl and NaOH can reach above 2 x 10(-10) and approximately 1 x 10(-10) respectively, which may be in the detection range of observational facilities such as ALMA and JWST. For warm-up models, we found that if we consider sodium-bearing molecules to be co-desorbed with water ice, then gaseous NaCl can reach a sufficiently large abundance for detection to be possible. However, more experiments and quantum calculations are needed to constrain the relevant reaction rates in our simulations better.

References

[1] J. Cernicharo & M. Guélin, 1987, A&A 183, L10.
[2] S. N.Milam, A. J. Apponi, N.J. Woolf, & L. M. Ziurys, 2007, ApJ 668, L131.