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Transformation and sublimation of interstellar ices: insights from laboratory experiments and astronomical observations

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Publications

Refereed publications as lead author

1. *H_2S ice sublimation dynamics: experimentally constrained binding energies, entrapment efficiencies, and snowlines*
   Santos, J. C., Piacentino, E. L., Bergner, J. B., Rajappan, M., Öberg, K. I., 2025, Astronomy & Astrophysics, in press. (Chapter 5)

2. *Formation of carbonyl sulfide (OCS) via SH radicals in interstellar CO-rich ice under dense cloud conditions*
   Santos, J. C., Linnartz, H., Chuang, K.-J., 2024c, Astronomy & Astrophysics, 690, A24. (Chapter 6)

3. *SO_2 and OCS toward high-mass protostars: A comparative study between ice and gas*
   Santos, J. C., van Gelder, M. L., Nazari, P., Ahmadi, A., van Dishoeck, E. F., 2024b, Astronomy & Astrophysics, 689, A248. (Chapter 8)

4. *Formation of S-bearing complex organic molecules in molecular clouds via ice reactions with C_2H_2, HS, and atomic H*
   Santos, J. C., Enrique-Romero, J., Lamberts, T., Linnartz, H., Chuang, K.-J., 2024a, ACS Earth and Space Chemistry, 8, 1646. (Chapter 7)

5. *Interaction of H_2S with H atoms on grain surfaces under molecular cloud conditions*
   Santos, J. C., Linnartz, H., Chuang, K.-J., 2023b, Astronomy & Astrophysics, 678, A112. (Chapter 4)

6. *Resonant infrared irradiation of CO and CH_3OH interstellar ices*
   Santos, J. C., Chuang, K.-J., Schrauwen, J. G. M., Muiña, A. T., Zhang, J., Cuppen, H. M., Redlich, B., Linnartz, H., Ioppolo, S., 2023a, Astronomy & Astrophysics, 672, A112. (Chapter 3)

7. *Experimental confirmation of a new formation route to CH_3OH in interstellar ices: $CH_3O + H_2CO \rightarrow CH_3OH + HCO$*
   Santos, J. C., Chuang, K.-J., Lamberts, T., Fedoseev, G., Ioppolo, S., Linnartz, H., 2022c, The Astrophysical Journal Letters, 931, L33. (Chapter 2)

8. *Structure and stability of multiply charged naphthalene and its $C_{10}H_8$ isomers: bonding, spectroscopy, and astrophysical implications*
   Santos, J. C.[‡], Fantuzzi, F.[‡], Quitián-Lara, H. M., Martins-Franco, Y., Menéndez-Delmestre, K., Boechat-Roberty, H. M., Oliveira, R. R., 2022b, Monthly Notices of the Royal Astronomical Society, 512, 4669. (not included in this thesis)

[‡]These authors contributed equally

9. *A spectral survey of CH_3CCH in the Hot Molecular Core G331.512-0.103*
Santos, J. C., Bronfman, L., Mendoza, E., Lépine, J. R. D., Duronea, N. U., Merello, M., Finger, R. A., 2022a, The Astrophysical Journal, 925, 3. (Chapter 9)

10. *Rotational spectrum simulations of asymmetric tops in an astrochemical context*
Santos, J. C., Rocha, A. B., Oliveira, R. R., 2020b, Journal of Molecular Modeling, 26, 278. (not included in this thesis)

11. *Structure, stability, and spectroscopic properties of small acetonitrile cation clusters*
Cerqueira, H. B. A.[‡], **Santos, J. C.**[‡], Fantuzzi, F., Ribeiro, F. de A., Rocco, M. L. M., Oliveira, R. R., Rocha, A. B., 2020a, The Journal of Physical Chemistry A, 124, 6845. (not included in this thesis)

Refereed publications as co-author

1. *IR-induced CO photodesorption from pure CO ice and CO on amorphous solid water (ASW)*
Slumstrup, L., Thrower, J., Schrauwen, J. G. M., Lamberts, T., Ingman, E., Laurinavicius, D., DeVine, J., Terwisscha van Scheltinga, J., **Santos, J. C.**, Wenzel, G., Noble, J., McCoustra, M., Brown, W., Linnartz, H., Hornekær, L., Cuppen, H. M., Redlich, B., Ioppolo, S., 2025, ACS Earth and Space Chemistry, in press.

2. *Ammonium hydrosulfide (NH_4SH): a potential significant sulfur sink in interstellar ices*
Slavicinska, K., Boogert, A. C. A, Tychoniec, Ł., van Dishoeck, E. F., van Gelder, M. L., Navarro, M. G., **Santos, J. C.**, Klaassen, P. D., Kavanagh, P. J., Chuang, K.-J., 2025, Astronomy & Astrophysics, 693, A146.

3. *A systematic FTIR and VUV spectroscopic investigation of ion, electron, and thermally processed ethanolamine ice*
Zhang, J.[‡], Muiña, A. T.[‡], Mifsud, D. V., Kaňuchová, Z., Cielinska, K., Herczku, P., Rahul, K. K., Kovács, S. T. S., Rácz, R., **Santos, J. C.**, Hopkinson, A. T., Craciunescu, L., Jones, N. C., Hoffmann, S. V., Biri, S., Vajda, I., Rajta, I., Dawes, A., Sivaraman, B., Juhász, Z., Sulik, B., Linnartz, H., Hornekær, L., Fantuzzi, F., Mason, N. J., Ioppolo, S., 2024, Monthly Notices of the Royal Astronomical Society, 533, 826.

4. *Formation of N-bearing complex organic molecules in molecular clouds: ketenimine, acetonitrile, acetaldimine, and vinylamine via the UV photolysis of C_2H_2 ice*
Chuang, K.-J., Jäger, C., **Santos, J. C.**, Henning, Th., 2024, Astronomy & Astrophysics, 687, A7.

5. *Methane formation in cold regions from carbon atoms and molecular hydrogen*
Lamberts, T., Fedoseev, G., van Hemert, M., Qasim, D., Chuang, K.-J., **Santos, J. C.**, Linnartz, H., 2022, The Astrophysical Journal, 928, 48.

[‡]These authors contributed equally

Curriculum Vitae

I was born on the 17th of September, 1995, in Rio de Janeiro, Brazil, to an engineer mother and an astronomer father. Having a parent with a Bachelor's degree in astronomy is a rare privilege for a young science enthusiast, and I certainly took full advantage of it. My childhood was filled with long, lively conversations with my father about physics, astronomy, and the other fields within the natural sciences, and I remember waiting impatiently for the day I would finally get to study those subjects in school. But although astronomy was always a big part of my life, it was chemistry that ultimately stole my heart. That love began when I received a children's chemistry kit as a gift, which I used obsessively until every reagent was gone—at which point I cried inconsolably in frustration, devastated that I could no longer "do science".

My passion for STEM remained strong throughout my childhood and adolescence. I attended a traditional school in Rio de Janeiro, Colégio Santo Inácio, for both my primary and secondary education. There, I had the privilege of accessing well-equipped science laboratories, and hands-on STEM classes quickly became my favorite part of the curriculum. Still, I didn't realize that being a scientist could be a real profession—"that's something from the movies," my younger self thought, "certainly not something that exists here in Brazil." With that mindset, I decided to pursue a Bachelor's degree in chemical engineering, which at the time seemed like the ideal way to combine my passion for chemistry with a prestigious major that offered strong prospects for financial stability. I applied to the Federal University of Rio de Janeiro and was accepted.

The few years I spent studying chemical engineering were nothing short of dreadful. I had no interest—and frankly, no aptitude—for the industrial sector, and I found the chemistry portion of the curriculum far too superficial. At the same time, I began to notice that many of my professors were, in fact, scientists, which made me realize that science was, indeed, a viable career path. Around the same time, I also discovered the field of astrochemistry, which perfectly combined two of my greatest scientific passions: chemistry and astronomy. It was then that I mustered the courage and decided to fully commit to becoming a scientist. After three years studying chemical engineering, I resolved to transfer into the Chemistry major, scoring the highest grades in the transfer exam and securing the only available spot that semester. From there, I began seeking out supervisors for undergraduate research opportunities in astrochemistry.

I started my scientific career in laboratory astrochemistry, exploring vacuum cryogenic experiments on interstellar ice analogues. To pursue this project, I was awarded a two-years' undergraduate research scholarship. However, towards the end of my Bachelor's degree, I was also eager to explore other facets of astrochemistry, which led me to change topics for my final research project. Building on the results of my experimental work, I used computational chemistry methods to simulated the rotational spectra of molecules relevant to astrophysical environments. Both projects earned me several presentation awards at local as well as national conferences, and the latter

project also resulted in my first two first-author publications in peer-reviewed journals.

I then recognized that to become a well-rounded astrochemist, I needed to complement my education with a solid foundation in astronomy. With this goal in mind, I applied for the Master's program in Astronomy at São Paulo University—the largest university in Latin America, and one that I am immensely proud to be an alumna. As part of the admissions process, I was required to take a continent-wide graduate-level physics exam, which prompted me to independently study and fill the gaps in my chemistry-focused education. My efforts paid off when I scored above the 90^{th} percentile and was accepted into the program as the top-ranked candidate, also earning a graduate-level scholarship for the duration of my Master's degree. Excited for the challenge of living on my own for the first time, I left my hometown to pursue my Master's in São Paulo. During this period, I shifted my focus once again—this time, to observational astrochemistry—where I explored molecular emission lines in star-forming regions observed in submillimeter wavelengths.

After successfully defending my Master's remotely due to the COVID-19 pandemic, I started a PhD position with Prof. Dr. Harold Linnartz at Leiden University. Having explored various aspects of astrochemistry, I ultimately decided to return to experimental work, an area I've always found immensely satisfying. There's a special type of gratification in immersing yourself fully in the hands-on nature of experimental science. My laboratory endeavors extended beyond Leiden, with opportunities to conduct experiments at the FELIX Laboratory at Radboud University in Nijmegen, the Netherlands, as well as the ASTRID synchrotron light source and the low-temperature scanning tunneling microscope at Aarhus University in Denmark. Aarhus also served as the central hub for the InterCat consortium, which I was a part of throughout my doctorate. Additionally, I was fortunate to undertake a short-term research stay in Prof. Dr. Karin Öberg's lab at Harvard University, in the United States—a time that was particularly meaningful after the loss of my supervisor, Harold. Although the primary focus of my PhD was experimental, I have always maintained a passion for observations, so I continued pursuing observational research as a secondary field under the guidance of Prof. Dr. Ewine van Dishoeck.

The work conducted during my PhD culminated in this thesis and was presented at conferences around the world, including in Italy, Denmark, France, the United States, the Netherlands, Brazil, Spain, Iceland, and Japan. Concomitantly, I was the teaching assistant for the Bachelor's Research Project for three consecutive years, and have supervised two Master's students and co-supervised another Master's student. Following my defense, I will return to Harvard University to continue investigating the role of interstellar ices in the chemical evolution of star- and planet-forming regions—this time hosted by Prof. Dr. Karin Öberg as a 51 Pegasi b Fellow.

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There's something wry about how humans experience time—somehow, four years can feel like both a lifetime and the blink of an eye, all at once. My PhD journey was long and short, and not always easy, but looking back, I realize it was filled with moments of joy. These were only possible thanks to the people who supported, challenged, and inspired me along the way. Just as it takes a village to raise a child, it also takes a village to shape an independent researcher—and with this section, I'd like to thank mine.

The first person I'd like to thank is, sadly, no longer here to read this. Harold, thank you for offering me the incredible opportunity to work with SURFRESIDE^3, and for always being so supportive of me. You were right—I did get the prize fellowships I so deeply hoped for. I only wish you were here to know it.

Ewine, thank you for welcoming me so openly when I first reached out about pursuing an observational project; and again, for embracing me into your group with such generosity after we lost Harold. You have been an inspiration to me ever since I first discovered this amazing field we're in, and I'm deeply grateful to have had the opportunity to learn from your guidance.

Throughout my time in Leiden, I've met some incredible people. Katie, I'm so glad our paths crossed. You're a brilliant researcher and a wonderful friend. Thank you for making me feel less alone in this world. Brian—please don't cringe—you remind me so much of Luffy. Thank you for your friendship and for reminding me that it's okay to stand up for yourself. Fran, Nashanty, Yuan, your companionship has meant a lot to me. Jerry, I've always admired your big heart. Thank you for sharing your kindness and good humor with me. Will, you're one of the most steadfast people I know; I hope life brings you all the fulfillment you deserve. Martijn, Pooneh, and Łukasz, thank you for teaching me everything I know about ALMA observations. If I can now candidly call myself an observer, it's all thanks to you. To my fellow LfA folks—Carlos, Jeroen, Jessalyn, Ko-Ju, Marina, Martijn, Michał, Milan, Pranjal, Robin, and Thanh—thank you for the time we shared, I've learned a lot from you. Iara, Kelly, and Lina, thank you for teaching me what it means to be a supervisor. I hope I lived up to what you deserved. I'm also grateful to the astrochemistry community at Leiden for the many stimulating discussions: Andrew, Andrés, Ardjan, Joan, Lukas, Lucas, Logan, Margot, Marissa, Marten, Melissa, Marie, Mathilde, Milou, Serena, Thanja, Tobias, Tere, Xunchuan, and Zak.

To the InterCat team, thank you for opening so many doors for me. I'm sorry I don't have the space to name all of you. Signe, I'm so grateful for your friendship. Despite spending most of our PhDs apart, I've always felt close to you. I think I would've gone crazy watching the STM scan line by line without your company. Alfie, thank you for always making me laugh. Ale, you're one of the sweetest people I know, I'll never forget our epic chair race during our ASTRID beamtime.

Though I only spent five weeks at the CfA, I feel fortunate to have many people to

thank from my time there. Karin, thank you for welcoming me so warmly into your lab and for supporting me throughout postdoc applications. I've long admired your work, but after witnessing your dedication to your mentees, I've come to appreciate you even more on a personal level. Elettra, I truly admire your authenticity and your drive to support others. Alexandra, Alexia, Alice, Bea, Jenny, Marissa, Michelle, and Suchi, you are all powerhouses, and I've learned so much from you. Mahesh, having your support is a privilege that made all the difference in my experiments.

To my dojo, Daidokan, thank you for welcoming me with such inclusiveness. Being the only expat in a Dutch-speaking dojo felt daunting at first, but your warmth quickly put me at ease. I even ended up as treasurer! Thank you for your patience as I fumbled through figuring out what a voorziening was. Ilia sensei, Roek sensei, thank you for sharing some of your budo knowledge with me. To my fellow dojo mates—Esmée, Gabija, Iris, Julia K., Julia van V., Juul, Lisette, Marthe, Miriam, Nienke, Nikki, Noortje, Rosa, Sabina, Sandra, Sanne de J., Sanne de V., Saar, Thirza, and Yalda—thank you for making this space both challenging and safe, and for being such dedicated training partners. Though I'll be leaving Daidokan, karate will always be part of my life—and I have you all to thank for that.

Mom, dad, thank you for always being in my corner. Knowing I could always count on your safety net gave me the strength to take risks and keep going. To my in-laws—Sônia, Flávio, Camila, Juca, Caio, and Ciça—thank you for embracing me into the family. You're so much fun to be around, and I truly cherish our Sunday gatherings whenever we're back home.

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