High Pressure C₆₀S₈: A Well-Travelled Cool Structure

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Sometimes a structure becomes more than just a structure. In this case, it was also a cornerstone proof of something suspected, something indicated by other techniques, and it also was something that felt a bit like catching lightning in a bottle. This cool structure also carries with it the weight of the last five years: years marked by widely shared devastation, tragedy, mourning and resilience.

After an effervescent experience at IUCr 2017, sharing the story of these fullerene co-crystals at high pressure, I felt a renewed excitement to complete the tale. The spectroscopy indicated a high-pressure form that was quenchable to ambient pressure, but my experience had shown that pressurizing too high would lead to amorphization. I walked the delicate balance between reactivity and destruction, and was able to take an ambient pressure data collection on a crystal recovered from a DAC experiment. This was the summer of 2018, and I had just accepted a position at Diamond Light Source. I gleefully shared the preliminary structure with Marilyn Olmstead, my PhD advisor, academic mother and a primary crystallographic confidante. We both agreed that it was a nice result, a cool structure, and that we would discuss it further.

Moving internationally and taking a new position with management responsibilities definitely interfered with my ability to finalize this structure. Getting settled in a new country, navigating the pitfalls of a supposedly shared language and learning how to be a decent manager were my main priorities, and just when I was feeling like I had it all under control, there was a global pandemic. Marilyn and I stayed in sporadic but meaningful communication. We occasionally talked about the high pressure work, but it was not a priority in light of everything else that was going on. I will never forget hearing from her immediately after giving my talk at a virtual ACA 2020. I'm so proud of you, she wrote.

In the months following Marilyn's tragic passing, I found myself increasingly avoiding crystal structure refinements in general.Being a beamline scientist is a chaotic existence- the beamline always finds ways of demanding your time and energy. Being distracted away from crystallography was my best coping strategy for those dark times. Unfortunately, these fullerene samples were great for commissioning my fledgling single crystal high-pressure program, providing a constant reminder of the work that remained unfinished and unpublished. This cool structure languished on my computer, often opened, but rarely modified. Fast forward to today, I left Diamond late last summer, now back in California, working for Rigaku Americas and delicately dabbling in crystallography once more. ACA 2023 is swiftly approaching; I have a cool structure to share. Will this story end in triumph, with a beautifully modeled structure of a high-pressure phase recovered to ambient? Only one way to find out.