PUSHING THE SIZE LIMITS OF BROADBAND ROTATIONAL SPECTROSCOPY: THE SEVOFLURANE TRIMER

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The size of the attainable target systems for broadband rotational spectroscopy has been steadily increasing since its introduction in 2006. In 2013, we presented at this conference the characterization of the sevoflurane dimer. This complex represented, at that time, one of the larger systems observed through rotational spectroscopy. The collected spectrum exhibited a large dynamic range and many transitions remained unassigned. With the advent of newer, faster and more reliable conformation sampling tools like CREST and automated fitting routines such autofit and its implementation in Pgopher, we reassessed the ability of rotational spectroscopy to probe increasingly larger, heavier systems. In this talk we will present the observation of the sevoflurane trimer by chirped-pulse Fourier transform microwave spectroscopy, identified through the interplay of experimental and computational methods. The trimer (>600 Da), one of the largest molecular aggregates observed through rotational spectroscopy, showcases the potential of rotational spectroscopy to study larger biochemical systems but also uncovers the challenges ahead as the mass of the system increases. These will be presented and discussed.