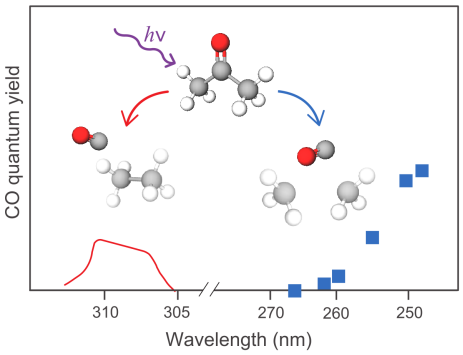
CO FORMATION FROM ACETONE PHOTOLYSIS: THE ROAMING PATHWAY

LORRIE S. D. JACOB, *Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, Cambridgeshire, United Kingdom*; KELVIN LEE, *Accelerated Computing Systems and Graphics, Intel Corporation, Hillsboro, OR, USA*; TIMOTHY SCHMIDT, KLAAS NAUTA, SCOTT KABLE, *School of Chemistry, UNSW, Sydney, NSW, Australia*.



Acetone is one of the most abundant ketones in the atmosphere, with 73 million tonnes emitted or formed in the atmosphere annually. Additionally, as the simplest ketone, understanding the photodynamics of acetone can improve our understanding of the photolysis pathways of other ketones.

CO formation from acetone photolysis was studied over the whole $S_1 \leftarrow S_0$ absorption spectrum,[a] however, this talk focuses on the longer wavelengths (305-320 nm). Resonance enhanced photoionisation (REMPI) and photofragment excitation (PHOFEX) of the CO photofragment at photolysis wavelengths longer than 300 nm, combined with laser-induced fluorescence (LIF) of acetone, found CO was forming from a unimolecular pathway, attributed to roaming. Although roaming is often associated with 'cold' rotational distributions, this does not seem to be the case for CO formed from roaming in acetone. The CO products had significant rotational excitation up to $J \sim 80$.

Fourier transform infrared spectroscopy was used to obtain quantum yields of the photolysis products of acetone from 285 – 325 nm at various pressures of synthetic air and nitrogen bath gas (3-760 Torr total pressure). Carbon monoxide was found to have a quantum yield of up to 10% in non-oxidative conditions at 3 Torr and 760 Torr. In an atmosphere of synthetic air at actinic wavelengths, this pathway was reduced to a maximum of 3%.

[a] Jacob, L.S.D.; Lee, K.L.K.; Schmidt, T.W.; Nauta, K.; Kable, S.H. *J. Chem. Phys.* **2022**, *156*, 094303