Minerals on Titan: the crystal structure of diacetylene

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Saturn's largest moon, Titan, is an important extra-terrestrial target for studying planetary chemistry and potential astrobiology. With an upper atmosphere rich in nitrogen and methane that undergoes conversion into hydrocarbons, nitriles and aerosols, this icy moon is a valuable model for investigating prebiotic chemistry analogous to early-Earth [1,2]. Among the larger molecules detected in Titan's atmosphere, diacetylene (C_4H_2) is of particular interest due to its significant absorption of photons at longer wavelengths, which facilitates the formation of radical species such as C_4H and C_4H_3 that are key to polycyclic aromatic hydrocarbon (PAHs) formation [3].

In this study, we combined powder X-ray and neutron diffraction, Raman spectroscopy and periodic-DFT calculations to characterise the crystal structure of diacetylene for the first time. The structure is described in the space group $P2_12_12_1$ with four molecules in the unit cell (Fig. 1). The diacetylene molecules are arranged in a layered structure dominated by CH•••π interactions, which leads to anisotropic thermal expansion behaviour. At ambient pressure, no structural phase transitions were observed in the 5–220 K temperature range. Due to its structural similarity with acetylene, diacetylene may serve as a potential co-crystal component of particular importance for Titan's surface chemistry and geomorphology. This is of potential importance in view of the upcoming NASA Dragonfly mission.

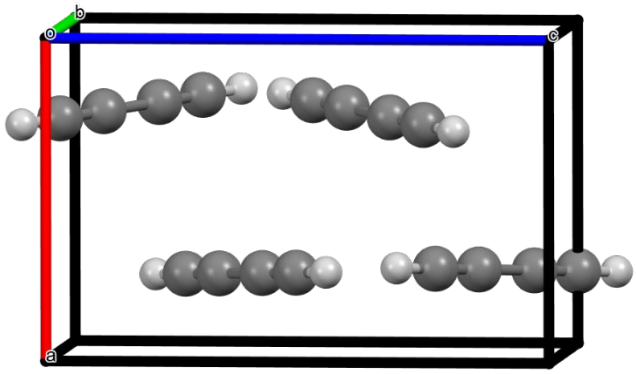

Figure 1. Representation of the structure of diacetylene refined in space group $P2_12_12_1$ against neutron powder diffraction data collected at 5 K.

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