

***Paxillus involutus* hyphae: Imaging their structure and interaction with mineral surfaces using AFM**

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Experiment

Plant and ectomycorrhizal interactions with minerals were investigated under axenic culture conditions. Chlorite and biotite flakes were inserted in an axenic microcosm depleted in Fe with *Pinus sylvestris* (Scots pine) colonised with the ectomycorrhizal fungus *Paxillus involutus*. Fungal hyphae structures on the mineral were imaged at the nanoscale.

Atomic Force Microscopy (AFM), operating in contact and tapping modes was used for topographic imaging, and pixel-by-pixel force spectroscopy, or force volume mapping, was used to build up adhesion and elastic moduli maps of the hyphae and surrounding mineral surface, to determine the physical properties of the fungal mineral surface interactions.

Fungal hyphae and the mineral surface were imaged after several months of fungal colonisation. Images were also taken after partial cleaning of the fungi from the mineral surface with gentle wiping, and after their complete removal, to record any fungal-induced changes on the mineral surface. The images have been correlated with Scanning Electron Microscopy (SEM), X-ray Photoelectron Spectroscopy (XPS) and other surface-sensitive techniques.

AFM images of fungal hyphae and a layer covering the surface are shown in Figure 1. Globular features covering the mineral surface were visible at the nanoscale on both chlorite and biotite, whereas geometrical patterns of approximately 4 nm in height and between 0.5 μm and 1 μm in width were only observed on the biotite. These were more pronounced after partial removal of the hyphae and the layer covering the surface.

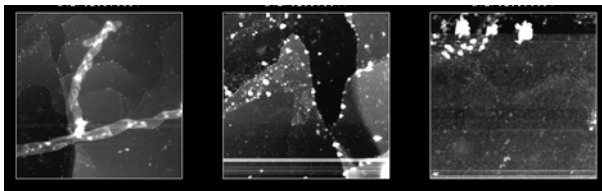


Figure 1: AFM images of a branching hypha (left) and layer on chlorite (Images field of view ranges from 40 μm to 4.21 μm , left to right)

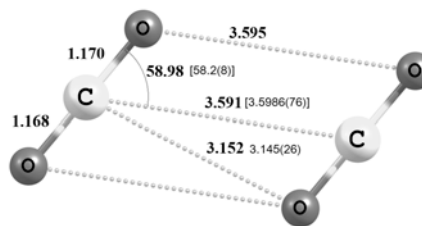
Thermodynamic and structural stability of $(\text{CO}_2)_n$ n=2-4: An *ab initio* and QTAIM Study

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Quantum chemical and experimental studies of weakly bound molecular complexes are of fundamental importance in shaping our understanding of molecular interactions in the condensed phase. The gas phase carbon dioxide clustering reaction according to $n(\text{CO}_2) = (\text{CO}_2)_n$ provides a suitable model for such studies and, can as such provide valuable insight into the stability of carbon dioxide clusters in the Earth's atmosphere, the occurrence of carbon dioxide clouds on Mars as well supercritical phenomena in the lower Venusian atmosphere [1]. The first experimental data on the CO_2 multimer series stems from microwave spectroscopic work at 1.6K, that revealed the existence of a slipped parallel C_{2h} symmetry for the carbon dioxide dimer [2]. Only one study exists where $(\text{CO}_2)_2$ bonding patterns, structures and their relationship to the theoretical binding energy have been discussed in detail [3]. Unfortunately, there are no reliable experimental thermodynamic data (Gibbs energy, enthalpy and entropy) for either the dimerization reaction or formation of higher clusters from starting CO_2 .

Here we report new CO_2 cluster structure parameters as well as new values for ΔG , ΔH and ΔS for $(\text{CO}_2)_n$ clustering reactions up $n=4$ building on both QTAIM and *ab initio* approaches at MP2/cc-pVTZ level of theory and atmospheric T. For instance, MP2 level $(\text{CO}_2)_2$ geometric parameters from this study are in excellent with microwave data (Figure below) [2]. The corresponding CO_2 dimerization enthalpy and entropy are $-1.5 \text{ kJ}\cdot\text{mol}^{-1}$ and $-70.7 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$, respectively, indicating that the dimer and higher clusters may be present in appreciable levels in the 60-80km altitude range of the Martian atmosphere and thus an important requirement for CO_2 cloud nucleation.



[1] Montmessin *et al*, 2006, *Icarus*, **183**, 403; [2] Jucks *et al*, 1988, *JCP*, **88**, 2185; [3] Bone *et al*, 1996, *JPC*, **100**, 10892.