

Dr. Tim Johnson  
Pacific Northwest National Laboratory, WA, USA

## **Sporulated and Vegetative Bacillus Bacteria Infrared Signatures: Chemical Assignments**

The unique infrared signatures of Bacillus bacteria can easily be used to identify such species, which are related to the pathogen B.anthraxis, even at distances. However, the origins and reproducibility of the IR bands depends on different parameters which are still under investigation. Our recent studies have used eight different Bacillus bacteria and have shown that there are distinct and strong IR bands associated with either the vegetative state or the sporulated state. Both states have strong signatures from the protein Amide I and Amide II bands, but the vegetative state is dominated by peaks associated with phospholipids. The sporulated cells have been shown to contain trace levels of these same signatures and we attribute these to vegetative (debris) amongst the spore cells. For the spore cells, we have clearly shown that many of the non-protein peaks arise from calcium dipicolinate trihydrate  $\text{CaDP}\cdot 3\text{H}_2\text{O}$ , including a distinct quartet of peaks at 766, 725, 701, and 659  $\text{cm}^{-1}$  that clearly are associated with  $\text{CaDP}\cdot 3\text{H}_2\text{O}$ . The vibrational peaks and effects of hydration were studied using quantum chemistry in the PQS software package showing the low frequency modes include contributions from the  $\text{Ca}^{2+}$  counterion and hydration waters including Ca-O-H bends, water - Ca-O torsions and O-C-O bends. The reproducibility of this quartet and other peaks adds much greater reliability and precision to the detection of bacterial spores.