Can you SQUEEZE an ion? And if not, why not?

William Clegg[1]

[1]Chemistry, School of Natural and Environmental Sciences, Newcastle Univ

bill.clegg@ncl.ac.uk

The SQUEEZE procedure of Ton Spek's software PLATON is a useful tool for dealing with highly disordered parts of a crystal structure for which a model using resolved atoms cannot be satisfactorily developed. It is most often used for disordered solvent, the chemical identity of which may or may not be known from the methods of synthesis and crystallisation. At times controversial, it is nowadays widely accepted as an appropriate approach. Its validity and applicability, however, are sometimes debated. One opinion voiced on some user group discussions is that SQUEEZE should not be used for charged species, leading to a structure in which there is charge imbalance in the defined refinement model. I will present one particular case in which the cations of a salt with well-defined polyoxometalate anions are so badly disordered in a high-symmetry space group that it is impossible even to begin locating atoms. Applying SQUEEZE to these tetraalkylammonium cations (and solvent that may also be present) gives a good result - unless the 'ban on SQUEEZE for ions' dictum is followed. I wonder how the audience will divide on this question!

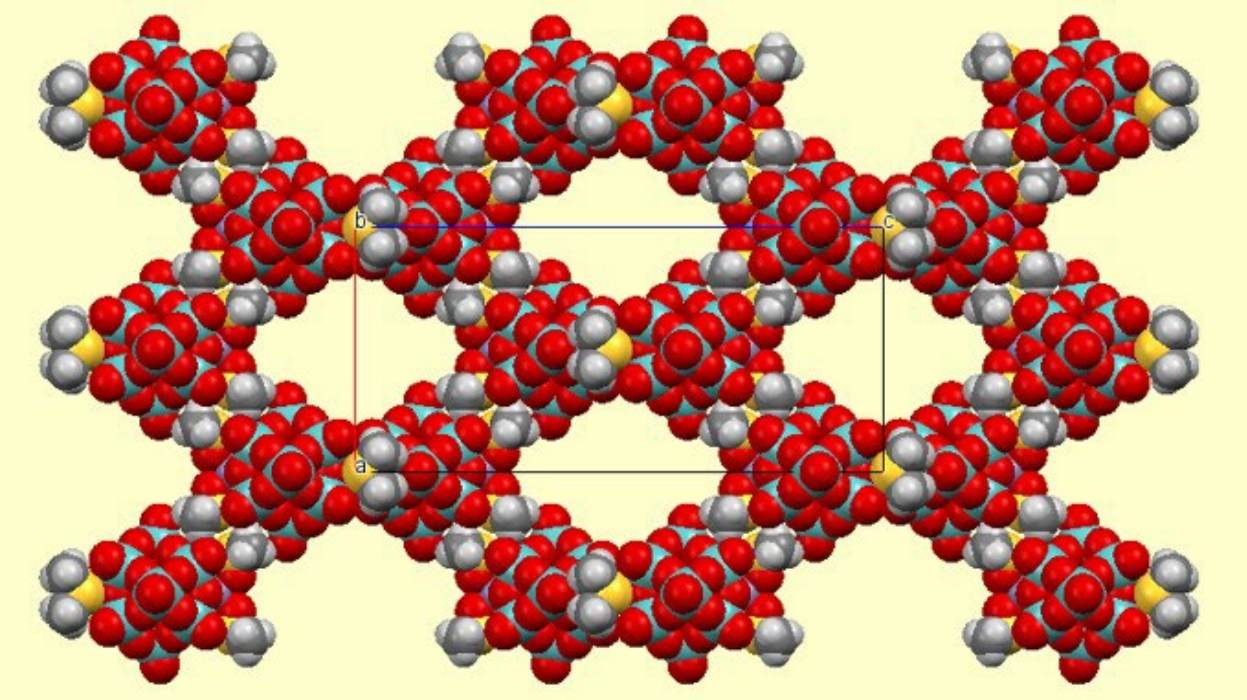

Figure 1