Z, Z' and Z" (or ZZZ….)

The value *Z, Z'* and *Z"* are often confused. What are these values and how do we use them. First let us look at *Z*.

Z

The value *Z* is defined as the number of "formula units" that are related by symmetry, in the unit cell. The "formula unit" can be described as the basic fundamental formula for the compound. For example, sugar has a molecular formula of $C_{12}H_{22}O_{11}$ and 2 molecules (of $C_{12}H_{22}O_{11}$) related by symmetry operations per unit cell in the crystalline state, therefore crystalline sugar has a $Z = 2$. For sugar the two molecules in the unit cell are related by a symmetry operation (a 2_1 skrew axis), therefore the number of unique non-symmetrically nonequivalent molecules in the unit cell of sugar is one.

Z" and Z'

For molecular solids of single neutral molecular compounds, that do not co-crystallize with included solvents, the number of crystallographic nonequivalent molecules in the unit cell has the value Z". If none of the molecules are found on special positions then Z"=Z' where Z'=Z/M (where M is the multiplicity of the general positions and Z is equal to the number of residuals in the unit cell). If the asymmetric unit contains more than one molecular unit the Z' will be greater than 1. For example if sugar crystallized with two non-symmetrically related molecules in the space group P1 (M=1) then the *Z* would equal one and $Z' = Z'' = 2$. Normally the value of Z' for crystals that contain more than one molecule in the asymmetric unit, is less four. A few of cases may be due to unnecessarily low symmetry and other sources of error. .