Theoretical lattice energies can be calculated for substances that do not exist or do not form ionic substances. For example theoretical lattice enthalpy values can be calculated for MgCl and $MgCl_3$. These theoretical values can be used in a Born- Haber cycle to calculate the theoretical value of the enthalpy of formation, ΔH_f for these lattices. This may tell us why these lattices do not form.

<u>The Pure ionic Model of ionic Compounds is not Always Entirely Correct</u>

If there is a large negative ion in the lattice, especially with a large charge, and a small positive ion with a large charge, then the negative ion may be polarised. The positive ion may attract part of the negative charge of the ion towards itself. This will distort the shape of the ion, polarisation occurs indicating the bond contains some covalent character.

For the halides of Alkali metals, the theoretical values are similar to the experimental;

- Simple ionic model is suitable and acceptable
- Ions are spherical with uniformly distributed charge
- Ionic crystals have strong character

For silver halides, large discrepancies exist between the values. The experimental values are greater than the theoretical values;

- Simple ionic model is inaccurate for AgX
- Ions are not completely spcherical
- Bonding is stronger than expected. This is because the bonding is partially covalent and the electron density between the nuclei of the bonded ions is higher and extra bonding exists. Electron transfer from metal to non- metal is incomplete.

Summary

- Good agreement means that the crystals are essentially ionic in nature
- Poor agreement means that considerable covalent character exists in the ionic crystal, the ionic bond is polariesd