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On symmetry relationships of binary metallic graphite intercalation compounds structure family - understanding staging transition mechanism and a helpful tool for neutron diffraction studies

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Graphitic materials have historically a huge technological importance due to their manifold interesting properties, which mostly arise from the anisotropic bonding arrangement. The weak interlayer bonding opens the capability for intercalation reactions and formation of graphite intercalation compounds (GICs), of special interest are the binary metallic GICs, which are well-known in two families of compounds, MC6 and MC8. Additionally, the high reversibility of the intercalation reaction made graphite-based anode materials commonly used in lithium-ion batteries (LIBs). We reviewed all existing binary stage-1 GIC structure reports from the ICSD-database and other sources and explore the symmetry relationships of these structures by applying group-subgroup considerations. This review gives new insights on the structure building forces in GICs and adds a new view on the phase transition mechanisms between intermediate stages for GICs depicted in the family tree. This can improve detailed neutron diffraction analysis as it helps to identify the structural origins of small deviations in diffraction patterns easily, based on the symmetry relationships of the crystal structures and help to control aging and cell performance characteristics in the Li-GIC system in LIBs, since despite very detailed neutron diffraction studies, still many open questions remain in the complex Li-GIC system.

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