

The structure of Chalcopyrite (CuFeS_2)

The crystal structure of chalcopyrite is defined within a body-centered tetragonal (quadratic) lattice (I), composed of three motifs: copper (Cu), iron (Fe), and sulfur (S), giving it the chemical formula CuFeS_2 , or copper iron sulfide. The vertices, center, and faces of the parallelepiped are occupied by Cu atoms, while the Fe atoms are positioned at the midpoints of the edges along the oz -axis and within the faces of the parallelepiped.

The sulfur atoms are located inside the structure at the following coordinates: $(1/4 \ 1/4 \ 1/4)$, $(1/4 \ 1/4 \ 5/4)$, $(3/4 \ 1/4 \ 3/4)$, $(3/4 \ 1/4 \ 7/4)$, $(1/4 \ 3/4 \ 3/4)$, $(1/4 \ 3/4 \ 7/4)$, $(3/4 \ 3/4 \ 1/4)$, and $(3/4 \ 3/4 \ 5/4)$. This arrangement highlights the complex and ordered nature of the chalcopyrite crystal structure, which is significant in mineralogy and materials science due to its unique properties and applications

