

Calculated and Experimental Properties of the Perfect Crystal Lattices of
 $\text{Sr}_2\text{Fe}_2\text{O}_5$ and $\text{Sr}_4\text{Fe}_6\text{O}_{13}$

(a) Elastic Constants (GPa)

	$\text{Sr}_2\text{Fe}_2\text{O}_5$	$\text{Sr}_4\text{Fe}_6\text{O}_{13}$
c_{11}	281.2	307.2
c_{12}	113.1	123.4
c_{13}	63.6	75.7
c_{33}	269.4	308.3
c_{44}	91.2	106.3
c_{66}	59.2	108.6

(b) Dielectric Constants

	$\text{Sr}_2\text{Fe}_2\text{O}_5$	$\text{Sr}_4\text{Fe}_6\text{O}_{13}$
ϵ_0	7.12	12.02
ϵ_{inf}	2.16	2.32

Lattice energies for binary oxides

Formula Unit	Experiment ⁴⁵ (eV)	Simulation (eV)
FeO	-39.333	-40.15
Fe ₂ O ₃	-148.304	-147.66
SrO	-33.342	-35.72
CoO	-39.768	-40.85