Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Crystal and Local Structure Refinement in $Ca_2Al_3O_6F$ Explored by X-ray Diffraction and Raman Spectroscopy

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Table S1. Parameters of the interatomic interaction potential

Interaction	λ, aJ/Å^2	ρ, Å
Ca – O	240.17	0.3834
Ca – F	248.00	0.3834
Al – O	215.17	0.3734
Al – F	220.17	0.3800
F – F	230.17	0.3834
O – O	400.17	0.4000
O – F	250.17	0.3834

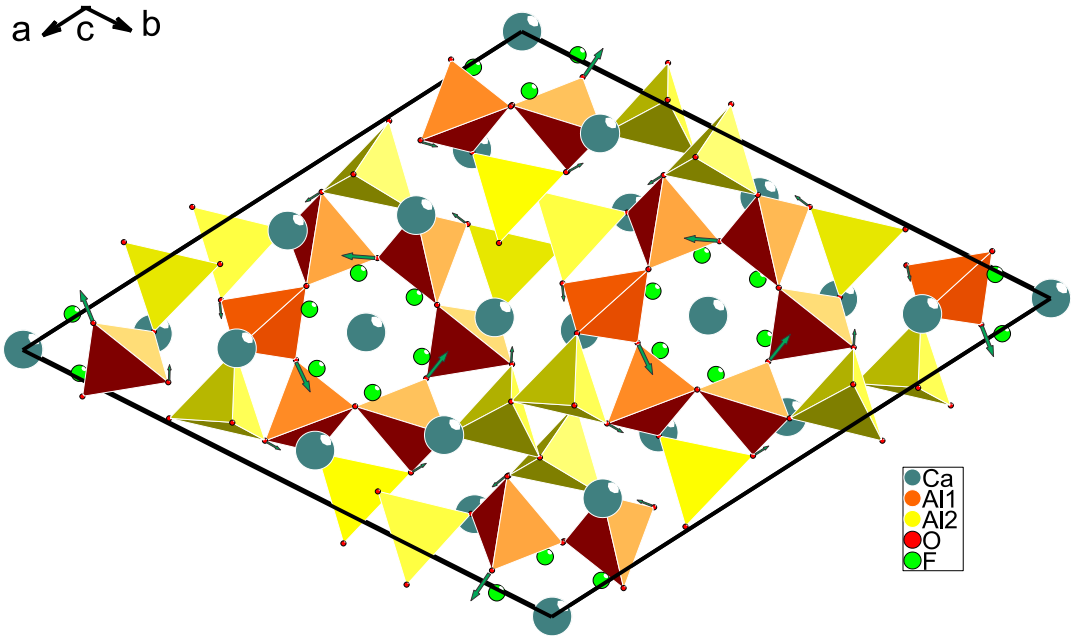

Fig. S1. A_g (797 cm^{-1}) vibrational mode of AlO_4 tetrahedrons.

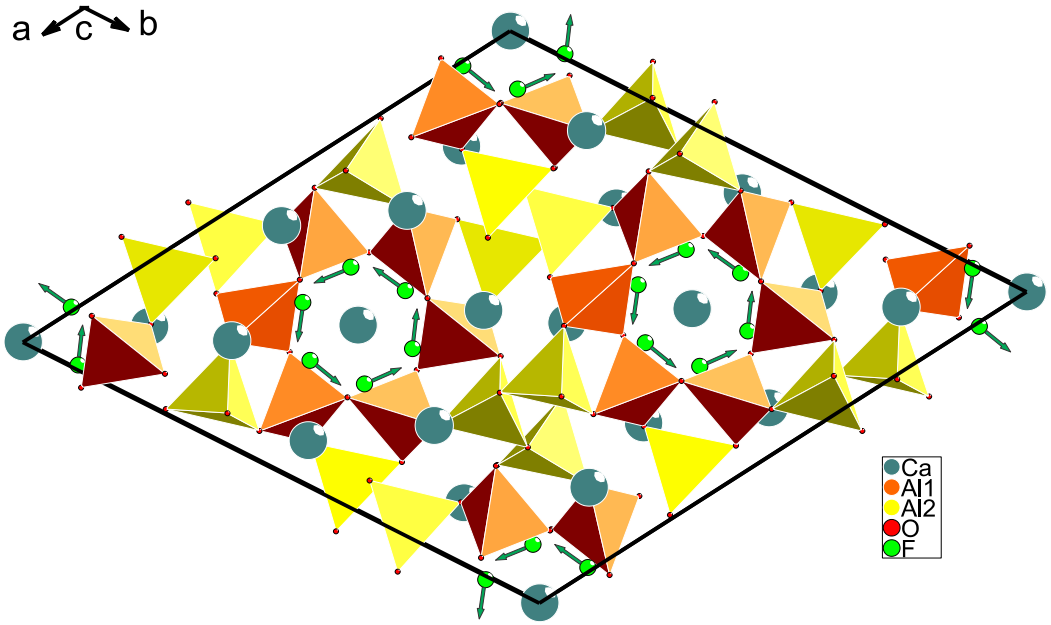

Fig. S2. A_g (252 cm^{-1}) vibrations mode of fluorine in $Ca2O_3F_4$ polyhedrons.