Raman investigation of $Ca_5(SiO_4)_{1.5}(SO_4)_{1.5}(OH,F)$ - $Ca_5(AsO_4)_3(OH,F)$ - $Ca_5(PO_4)_3(OH,F)$ series from calc-silicate xenoliths of the Upper Chegem caldera, Northern Caucasus, Russia

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Minerals belonging to the ellestadite–johnbaumite–svabite–apatite solid solution are wide spread in skarn xenoliths within ignimbrites of the Upper Chegem caldera in the Northern Caucasus, Russia. Mineral association (larnite, rankinite, wadalite, rondorfite etc.) indicates high temperature and low pressure conditions of formation, corresponding to the sanidinite metamorphic facies [1].
In the present work hydroxylellestadite $(Ca_{4.98}Na_{0.02})_{\sum 5}[(SiO_4)_{1.42}(SO_4)_{1.09}(CO_3)_{0.38}(PO_4)_{0.11}]_{\sum 3}[(OH)_{0.77}Cl_{0.14}F_{0.12}O_{0.06}]_{\sum 1}$, arsenate hydroxylellestadite $Ca_5[(SiO_4)_{1.28}(SO_4)_{1.05}(AsO_4)_{0.44}(CO_3)_{0.18}(PO_4)_{0.05}]_{\sum 3}[(OH)_{0.74}Cl_{0.15}F_{0.06}\square_{0.05}]_{\sum 1}$ and svabite $(Ca_{4.96}Na_{0.04})_{\sum 5}[(AsO_4)_{1.67}(PO_4)_{0.54}(SiO_4)_{0.38}(SO_4)_{0.36}(VO_4)_{0.04}(CO_3)_{0.01}]_{\sum 3}[F_{0.67}(OH)_{0.23}Cl_{0.06}\square_{0.04}]_{\sum 1}$ Raman spectra has been compared. The main bands on Raman spectrum of hydroxylellestadite are following: SiO_4^{4-} (ν_1) 855 cm^{-1}, (ν_2) 327 cm^{-1}, (ν_4) 530 cm^{-1}; SO_4^{2-} (ν_1) 1004 cm^{-1}, (ν_2) 466 cm^{-1}, (ν_3) 1137 cm^{-1}, (ν_4) 643 and 624 cm^{-1}; PO_4^{3-} (ν_1) 958 cm^{-1}, (ν_2) 429 cm^{-1}, (ν_4) 564 cm^{-1}. Characteristic for AsO_4^{3-} symmetric stretching bands vibrations [2] in arsenate hydroxylellestadite are overlap with (ν_1) SiO_4^{4-} in the range 840-860 cm^{-1}. Fitting results show bands (ν_1) SiO_4^{4-} for hydroxylellestadite at 855 cm^{-1} and (ν_1) AsO_4^{3-} for svabite at 853 and 831 cm^{-1}. AsO_4^{3-} vibration bands reveal at 953 cm^{-1} and 350 – 450 cm^{-1} and they overlap with (ν_1) and (ν_2) PO_4^{3-} for arsenate hydroxylellestadite. The band at 1074 cm^{-1} for ellestadite mineral group, has been interpreted as symmetric stretching of CO_3^{2-} vibrations [3,4]. Bands corresponding to the OH-stretching vibrations are noted in 3400 - 3700 cm^{-1} region of As-bearing ellestadite group minerals Raman spectra.

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