Structure refinements and crystal chemistry of palenzonaite garnet (Ca2,Na)M2V3O12 (M=Mg,Mn,Cu,Zn)

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The structural variation of parenzonaite garnet (Ca2,Na)M2V3O12 (M=Mg,Mn,Cu,Zn) is discussed based on the crystal structures obtained by determination of anisotropin temperture factors. These garnet type compounds exhibit interesting physical and chemical properties. Single crystals of (Ca2,Na)M2V3O12 (M=Mg,Mn,Cu,Zn) garnet were synthesized. The final R factors for each specimen were 0.01-0.03. The space group of these garnet type compounds is Ia3d at ambient condition. On the basis of the results obtained from structure refinements, geometric analyses of the polyhedral distortion were carried out. The cation-cation repulsion across the polyhedral shared edges is significant.