Crystal structures of $Rb_2(C_2O_4)\cdot H_2O$ and $Tl_2(C_2O_4)$: application of valence matching rule

Takuya Echigo[a], Mitsuyoshi Kimata[b], Atsushi Kyono[b], [a]*Course of Geoscience, Master's Program in Science and Engineering, University of Tsukuba.* [b]*Earth Evolution Sciences, Graduate School of Life and Environmental Sciences, University of Tsukuba.* E-mail: echigo@arsia.geo.tsukuba.ac.jp

Crystal structures of $Rb_2(C_2O_4)\cdot H_2O$ (monoclinic, space group $C2/c$, a = 9.617(6)Å, b = 6.353(5)Å, c =11.010(8)Å, β = 109.46(3)°, V = 634.2(8)Å^3, Z = 4, $R1$ = 0.026, for 2646 reflections) and $Tl_2(C_2O_4)$ (triclinic, P-1, a = 6.623(4)Å, b = 6.674(3)Å, c =5.854(4)Å, α = 90.031(35)°, β = 89.967(36)°, γ = 80.745(40)°, V = 255.3(3)Å^3, Z = 2, $R1$ = 0.082, for 1499 reflections) were determined using an imaging-plate diffractometer and a four-circle diffractometer, respectively (Mo$K\alpha$ radiation, graphite monochromator).

Incorporation of rubidium cations (Rb^+) with oxalic anions anions ($C_2O_4^{2-}$) establishes two-dimensional layer structure; water molecule $(H_2O)^0$ intercalates into the layers. Conformation of thallium cations (Tl^+) to seven oxygen atoms of oxalic anions sets up the two-dimensional layer structure, which is similar with that of rubidium oxalate. Except for water molecule, thallium oxalate is isotypic to rubidium oxalate (this study) and potassium oxalate $K_2(C_2O_4)\cdot H_2O$[1].

Bond valence analysis of these compounds reveals that $(H_2O)^0$ moderates the Lewis basicity of oxalic anion ($C_2O_4^{2-}$: 0.167). This moderated Lewis basicity matches the Lewis acidity of potassium and rubidium cation (K^+: 0.126, Rb^+: 0.124)[2], respectively: the valence-matching principle is satisfied.

[1] Sequeira A., Srikanta S., Chidambaram R. *Acta Cryst.,* 1970, **B26**, 77. [2] Brown I. D. *Acta Cryst.,* 1988, **B44**, 545.

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