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Influence of Lattice Interactions on Jahn-Teller Distortion of $[Cu(H_2O)_6]^{2+}$: The Crystal Structures of $K_2[Cu(H_2O)_6](SO_4)_{2x}(SeO_4)_{2-2x}$. Charles J. Simmons[1], H. Stratemeier[2], M.A. Hitchman[2], M.J. Riley[3], [1]Natural Sciences Div., Univ. of Hawaii at Hilo, Hilo, Hawaii, [2]School of Chemistry, Univ. of Tasmania, Hobart, TAS, Australia; [3]Chemistry Dept., Univ. of Queensland, St. Lucia, Queensland, Australia.

The Tutton salts form a series of isomorphous compounds crystallizing in the monoclinic space group $P2_1/a$ (Z = 2) having the formula $X_2[M(H_2O)_6](YO_4)_2$ (X = monovalent cation; M = a divalent cation; and Y = S or Se). The $[M(H_2O)_6]^{2+}$ cations possess C_i site symmetry. Of the first-row transition metals, only those with M = high-spin Cr^{2+} (^5E_g) and Cu^{2+} (^2E_g) are Jahn-Teller active, and, generally, two of the three M-O bond lengths are temperature dependent. The temperature dependence of the structure of the mixed-anion Tutton salt $K_2[Cu(H_2O)_6](SO_4)_{2x}(SeO_4)_{2-2x}$ has been determined for crystals with 0, 17, 25, 68, 78, 100% sulfate over a temperature range 80 to 325 K. For compounds with 0, 17, and 25% sulfate the long and intermediate Cu-O bonds occur to a different pair of water molecules from those with 68, 78, and 100% sulfate. A thermal equilibrium between the two forms is observed for each crystal. The temperature dependence of the Cu-O bond lengths has been analyzed using a model in which the JT potential surface of $[Cu(H_2O)_6]^{2+}$ is perturbed by a lattice-strain interaction. Significant deviations from Boltzmann behavior can be explained by cooperative interactions between neighboring complexes.