09.4.36 STRUCTURE OF A TWinned CRYSTAL OF WOLFFRAM's RED SalT [Pt(CsHsN)4]Cl2,Cl2 [Pt(CsHsNH-NH2)4]Cl2 • H2O is a typical example of halogen-bridged one-dimensional mixed-valence complexes. The crystal is characterized by linear chains of alternate stacks of octahedral and square planar ions. Mis-stacks, however, occur within the chains; the structure can be thought to consist of averaged octahedral ions with half-weighted Cl atoms and to have a half-period chain axis. This subcell structure was reported as pseudo-tetragonal, the space group 14mm(Craven & Hall, Acta Cryst., 1961, 14, 475-480). We report a twinning of the crystal. The pseudo-tetragonal reflections with 20 split as illustrated in Fig. 1: the twinned crystal consists of four individuals, c being the twin axis of 2 rotations. The structure was redetermined with intensity data of a twin component; monoclinic, the space group Im 21: a = 13.302(3), b = 13.337(5), c = 5.391(1) Å, β = 90.98(3)°. Fig. 2 shows a projection of the structure along c; Wolffram's red is isomorphous with the bromo analogue Reihlen's green(Brown & Hall, Acta Cryst., 1976, B32, 279-281).

Fig. 1. hk0.