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Phase transitions in K2Cr2O7 and structural redeterminations of phase II PETER WU, Southern Oregon University, T.J.R. WEAKLEY, E.R. YLVISAKER, R.J. YAGER, J.E. STEPHENS, R.D. WIEGEL, M. MENGIS, M.R. BAUER, PANOS PHOTINOS, SIDNEY ABRAHAMS — The phase transition in $K_2Cr_2O_7$has been studied and speculated upon inconclusively since 1908. We show that crystals of phase II with space group P, as grown from aqueous solution, undergo a first-order transition to phase I, space group $P2_1/n$, at $T_{PT} = 544(2)$ K on first heating. T_{PT} on cooling is 502(2) K; on subsequent heatings, $T_{PT} = 531(2)$ K, 502(2) on cooling. The mass loss between ∼531 and 544 K is identified as water that increasesT_{PT} on first heating due to the pressure of superheated water in inclusion defects. The structure of phase I that we inferred has been investigated by high temperature powder diffractometry, that of phase II independently redetermined by single crystal diffractometry. The details of the large rotations of atomic groups as symmetry elements are gained or lost at the first order phase transition will be discussed. A first order transition between the recently discovered phase IIb and that of phase I is likely but not between phases II and IIb. An intermediate phase may exist between phases IIb and I. **Financial support by National Science Foundation (DMR-9708246, DMR-0137323)**

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