atoms at distances of $\frac{1}{4}c$; however, Nd(2) is surrounded octahedrally by six O atoms from Si_2O_7 units. K(3) ions are between the Si_2O_7 units along $0,\frac{1}{3},z$. The K–O distances are longer than the sum of ionic radii of K and O (2·7 Å). All Nd–O polyhedra are isolated from each other with no bridging O atoms between Nd atoms. Therefore concentration quenching will be reduced in this compound. It has been shown (Hong & Dwight, 1974) that laser action is determined by the probability of electric-dipole transitions between certain orbitals of Nd^{3+}, which is highly dependent on the deviation from inversion symmetry around the Nd ion. Based on this argument, Nd(1) cannot produce laser action because it has $\bar{1}$ symmetry. However, Nd(2) could produce strong laser action because it is at a site with 32 symmetry.

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Cubic Structure of Chromium Iodine Boracite

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Abstract. $Cr_3B_7O_{13}I$, $M_r = 566{\cdot}56$, cubic, $F\bar{4}3c$, $a = 12{\cdot}214\ (1)$ Å, $V = 1822{\cdot}1\ (5)$ Å^3, $Z = 8$, $D_x = 4{\cdot}130$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 2·44 mm^{-1}, $F(000) = 2112$, $T = 298$ K, final $R = 0{\cdot}023$ for 109 unique reflexions with $I \geq 3\sigma(I)$; shortest interatomic distances (Å): [Cr–O] = 2·075 (2), [Cr–I] = 3·0520 (2), [O–B] = 1·439 (3), [O–O] = 2·393 (3). The deviation from planarity of the O-atom environment around the metal atom is compared with those of other cubic boracites.

Introduction. Boracites, $M_3B_7O_{13}X$ (M = bivalent metal ion, X = halogen ion), tend to undergo structural phase transitions (Schmid, 1965; Nelmes, 1974; Toledano, Schmid, Clin & Rivera, 1985). A structural feature of particular interest is the environment of the metal ions because it is relatively invariant with respect to the substitution of other metal and halogen ions whereas it changes strongly during phase transitions. In the cubic high-temperature modification the metal ions are surrounded by a deformed square-planar oxygen-ion configuration whereas in the trigonal, orthorhombic and monoclinic low-temperature modifications a halogen atom joins the coordination sphere thus leading to a fivefold, approximately square-pyramidal, non-metal configuration (Nelmes, 1974; Ito, Morimoto & Sadanaga, 1951; Abrahams, Bernstein & Svensson, 1981; Rivera, 1978). Despite extensive structural work (for reviews see Nelmes & Thornley, 1974; Nelmes & Hay, 1981) the reasons for this abrupt change in coordination are not yet clear.

The purpose of this study was to refine the cubic structure of a further member of this series and to compare its metal environment with those of other cubic boracites. Chromium iodine boracite, $Cr_3B_7O_{13}I$ (hereafter Cr–I), which remains cubic down to at least 4 K, appeared to be a favorable compound for such a comparison because structure data are available for its chlorine-based congener $Cr_3B_7O_{13}Cl$ (Nelmes & Thornley, 1974).

Experimental. Cubic crystals (edge length ≃0·05 mm) of blue-green colour were obtained by a gas-phase transport technique (Schmid, 1965; Schmid & Tippmann, 1979). Data collection: Philips PW1100 diffractometer, graphite monochromator, one hemi-

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$) *at* 298 K

$U_{eq} = \frac{1}{3}$ trace U.

	Wyckoff notation	x	y	z	U_{eq}
Cr	24(*c*)	0	2500	2500	63 (1)
I	8(*b*)	2500	2500	2500	71 (1)
B(1)	24(*d*)	2500	0	0	78 (1)
B(2)	32(*e*)	795 (2)	795 (2)	795 (2)	77 (1)
O(1)	8(*a*)	0	0	0	61 (1)
O(2)	96(*h*)	195 (1)	966 (2)	1795 (1)	46 (1)

sphere ($-17 \le h,k \le 17$), $[(\sin\theta)/\lambda]_{max} = 0{\cdot}6999$ Å^{-1}; 2111 integrated intensities, ω–2θ scan, scan width 1·3°, scan speed 0·03° s^{-1}, three standard reflections measured after every 120 min; maximum intensity change 3·6%, Lorentz and polarization corrections, no absorption correction ($\mu R = 0{\cdot}22$), lattice parameter determined from 36 reflexions in the 2θ range between 6 and 60°; structure refinement: space group and preliminary positional parameters from $Cr_3B_7O_{13}Cl$, full-matrix least squares, function minimized $\sum w(|F_o| - |F_c|)^2$, unit weights; scattering factors for neutral atoms and anomalous-dispersion corrections (*International Tables for X-ray Crystallography*, 1974), 21 parameters refined [one scale factor, four positional and 14 anisotropic thermal parameters, one isotropic extinction and one absolute structure parameter (Flack, 1983)], by using the *XRAY*76 system of programs (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976). Of 116 unique reflections, 7 were 'less-thans' [$I \le 3\sigma(I)$] and did not contribute to the refinement. Final R (wR) = 0·023 (0·031), for 109 contributing reflections. $(\Delta/\sigma)_{max}$ = 0·011. Standardized atomic parameters (Parthé & Gelato, 1984) are summarized in Table 1.* The refined value for the absolute structure parameter was 1·0 (1).

Discussion. The metal ions in cubic Cr–I boracite occupy a site of point symmetry $\bar{4}$ and have four nearly coplanar oxygen ligands at a distance of [Cr–O(2)] = 2·075 (2) Å, while the distance to their two halogen neighbours is much longer [Cr–I] = 3·0520 (2) Å. Both types of distance are longer than the corresponding distances in Cr–Cl boracite {[Cr–O(2)] = 2·055 (2), [Cr–Cl] = 3·033 (1) Å, at 291 K (Nelmes & Thornley, 1974)}, as expected from the larger cell parameter of Cr–I [a = 12·214 (1) Å] compared with that of Cr–Cl [a = 12·132 (3) Å]. On the other hand, structural details such as the planarity of the CrO_4 group cannot be rationalized in a simple way as shown in Fig. 1, in which the deviation from planarity, ε [for definition see Nelmes & Thornley (1974)], is plotted as a function of the cubic-cell parameter for various structurally characterized boracites: Cr–Cl (Nelmes & Thornley, 1974), Cr–I (this work), Co–I (Nelmes & Hay, 1981), Ni–I (Nelmes & Thornley, 1976), Cu–Cl (Thornley, Nelmes & Kennedy, 1976), Cu–Br (Nelmes & Hay, 1981), and Cu–I (Berset, Depmeier, Boutellier & Schmid, 1985). All data refer to room temperature except for Cu–Cl which refers to T = 390 K. Although the data show an overall trend which suggests that these units become more planar as the cell parameter decreases, the correlation is relatively poor. This can be seen, for example, from the three structural pairs Cr–Cl and Cr–I, Cr–I and Co–I, and Ni–I and Cu–I, which each have about equally planar MO_4 units but different cell parameters. While the compounds forming the first pair differ mainly with respect to the size of the halogens, those forming the latter two pairs differ mainly with respect to the electronic configuration of the transition metal ions (d^4, d^7, d^8 and d^9, for Cr, Co, Ni and Cu, respectively). This suggests that the detailed geometry of the MO_4 units in cubic boracites depends in a complex manner on both geometric factors, such as the size of the halogen atoms, and electronic factors, such as the electronic configuration of the metal ions.

The boron–oxygen framework in Cr–I does not differ much from that in Cr–Cl, as can be seen from a comparison of their interatomic distances (Å): [O(1)–B(2)] = 1·682 (2) and 1·683 (3), [O(2)–B(1) =

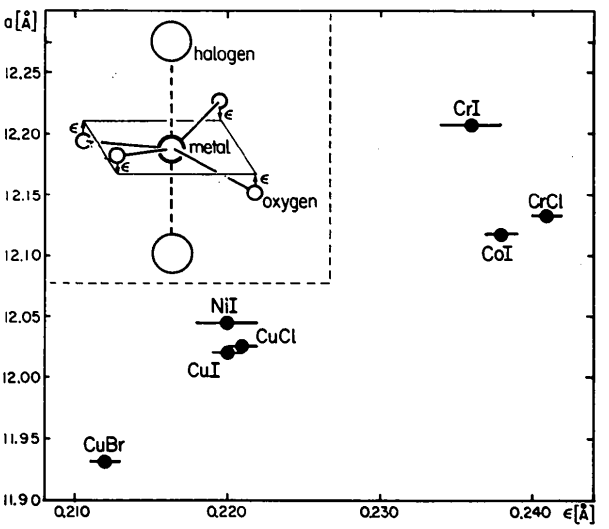

Fig. 1. Deviation from planarity, ε (for definition see insert), of the O-atom environment around the metal atoms in cubic boracites as a function of cell parameter, a. Except for Cu–Cl (T = 390 K), all data refer to room temperature. Site symmetry of metal atoms $\bar{4}$.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43821 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

1·479 (2) and 1·465 (1), [O(2)–B(2)] = 1·439 (3) and 1·436 (3), for Cr–I and Cr–Cl, respectively. The shortest separation between the oxygen atoms occurs within the BO_4 group {[O(2)–O(2)] = 2·393 (2) Å for Cr–I and 2·388 (2) Å for Cr–Cl}. As expected from the topology of the structure and the bonding, the metal ions vibrate mainly along the fourfold axes [$\langle u^2\rangle_{\parallel} = 0{\cdot}0109$ (3), $\langle u^2\rangle_{\perp} = 0{\cdot}0040$ (3) Å^2], *i.e.* in directions approximately perpendicular to the metal–oxygen bonds, and towards the nearest halogen neighbours (Fig. 1). These are the directions of greatest atomic shift during the structural phase transitions in boracites which lead from cubic to lower symmetry.

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Structure of a New Adduct Between Telluric Acid and a Condensed Phosphate: $K_4P_4O_{12}.Te(OH)_6.2H_2O$

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Abstract. Tetrapotassium *cyclo*-tetraphosphate–tellurium hexahydroxide–water (1/1/2), $M_r = 737{\cdot}96$, monoclinic, $C2/c$, $a = 9{\cdot}731$ (5), $b = 11{\cdot}43$ (1), $c = 17{\cdot}16$ (1) Å, $\beta = 99{\cdot}45$ (5)°, $V = 1883$ (2) Å^3, $Z = 4$, D_m not measured, $D_x = 2{\cdot}598$ Mg m^{-3}, $\lambda(Ag K\bar{\alpha}) = 0{\cdot}5608$ Å, $\mu = 1{\cdot}51$ mm^{-1}, $F(000) = 1432$, $T = 293$ K, final R value 0·024 for 2353 independent reflexions. Planes of $Te(OH)_6$ groups at $z = 0{\cdot}0$ and 0·5 alternate with planes of P_4O_{12} ring anions at $z = 0{\cdot}25$ and 0·75. The set of hydrogen bonds, which involves H_2O molecules as well as P_4O_{12} and $Te(OH)_6$ groups, spreads in a one-dimensional way along the **b** direction. The P_4O_{12} rings have twofold symmetry.

Introduction. Telluric acid has the property to form adducts with many kinds of inorganic phosphates, condensed or not. Up to now only one example of an adduct between $Te(OH)_6$ and an alkali *cyclo*-tetraphosphate has been reported: $2Te(OH)_6.(NH_4)_4P_4O_{12}.2H_2O$ (Durif, Averbuch-Pouchot & Guitel, 1982). In the present work we describe the second example of an adduct between telluric acid and an alkali *cyclo*-tetraphosphate: $K_4P_4O_{12}.Te(OH)_6.2H_2O$.

Experimental. $Te(OH)_6.K_4P_4O_{12}.2H_2O$ is readily prepared by slow evaporation at room temperature of a solution of potassium tetrametaphosphate and telluric acid with an approximate molar ratio 1/1. Large monoclinic prisms up to 5 mm in length are obtained after some days of evaporation.

Crystal size: 0·32 × 0·24 × 0·24 mm; Philips PW 1100 diffractometer; graphite monochromator; systematic absences: hkl $(h + k = 2n)$, $h0l$ $(h = 2n, l = 2n)$; 16 reflexions $(11 < \theta < 14°)$ for refining the unit cell; ω scan; scan speed: 0·02° s^{-1}; scan width: 1·20°; total background measuring time: 20 s; intensity and orientation reflexions: 800 and $\bar{8}00$; θ range: 3–27°; 3423 reflexions measured $(\pm h,k,l)$; $h_{max} = 15$,

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