spectrum ICDW, Eq. (1). Figure 3(b) gives the time evolution of the radial amplitude profiles, indicating localization of the instability. The typical diffusion density profile leads to higher drift velocity at the edge of the plasma [resistance $R(r) = \text{const}$; $j(r) = \text{const} = en(r)u(r)$]. The instability therefore develops from the periphery of the plasma. We also note that spatial growth in the axial direction inside the plasma column can be observed, showing that the end-plate sheaths do not contribute to wave growth.

Several important conclusions arise from this work. First, the current- and non-current-driven ICDW, far beyond onset, exhibit continuous ion-sound-like spectra and high growth rates. Second, these ion-sound-like instabilities can be excited in plasmas which are ion-sound stable, $T_e < T_i$: Since $\omega/k_z \gg v_i$, ion Landau damping is excluded. Third, work in progress indicates this instability as a new mechanism for the generation of strong anomalous resistivity and intense ion heating.

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[12] In a time-evolution sequence, the linear stage must appear before nonlinear effects. Since the discrete wave does not occur in pulsed operation, the continuous-frequency mode must exist by itself and cannot be a nonlinear stage of the (nonexistent) discrete linear mode.

New Structural Findings from a Neutron-Diffraction Study of One-Dimensional $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$*

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We report a single-crystal neutron-diffraction structure study of $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$ (KCP). Contrary to previous x-ray results we find that KCP is *non*centrosymmetric (space group $P4mm$ rather than $P4/mmm$). New water-molecule positions have been derived. The $Pt(CN)_4^{-2}$ groups are not precisely planar, the K^+ ions occupy ordered sites, and two crystallographically different Br^- ion sites are observed. The possible relationship of the Br^--ion disorder to the diffuse x-ray scattering previously observed is discussed.

The properties of the mixed-valence square-planar platinum compounds such as $K_2Pt(CN)_4Br_{0.3}\cdot 3H_2O$ (KCP) have attracted great interest because of their so-called one-dimensional metallic character.[1] The interpretation of the various measured properties has relied heavily on the detailed x-ray analysis of Krogmann and Hausen.[2] They found KCP to be composed of planar $Pt(CN)_4^{-2}$ groups which stack along the unique axis (tetragonal c) forming linear Pt-Pt chains with a metal-metal repeat distance of 2.89 Å, only ~0.1 Å greater than in the metal. Their proposed structure (centrosymmetric space group $P4/mmm$) requires disorder of the K^+ ion as well as the nonstoichiometric Br^- ion.

We wish to report the result of a full three-dimensional analysis of room-temperature neutron-diffraction data collected from a crystal of KCP. The newly derived structural parameters provide a much improved model for the interpretation of the electronic properties in terms of molecular structure. The crystals were prepared by the method of Saillant, Jaklevic, and Bedford.[3] We confirm that KCP conforms to the $4/mmm$ Laue group; the cell parameters are $a = 9.907(3)$ Å, $c = 5.780(2)$ Å, and $Z = 2$ in agreement with the x-ray findings. A search for superlattice reflections gave no evidence for a larger cell. A total of 1282 Bragg reflections ($\lambda = 1.142$ Å) were measured on an automated neutron diffractometer at the Argonne National Laboratory CP-5 reactor (temperature 22 ± 2°C). Averaging over equivalent groups yielded 565 independent data for the subsequent structure analysis. The x-ray coordinates and space group provided the initial structure model which on Fourier and least-squares refinement led to revised oxygen locations and approximate hydrogen-atom positions with the remaining atoms unchanged. However, a satisfactory, converged refinement was not obtainable and the lowest R factor[4] derived by using $P4/mmm$ was 0.103. A careful examination of Patterson and Fourier maps cast serious doubts on the K^+ and H_2O-molecule positions and, in turn, on the choice of the space group. Further analysis was then attempted using the alternative noncentrosymmetric space groups $P\bar{4}m2$, $P\bar{4}2m$, $P422$, and $P4mm$. The choice of $P4mm$, which provides ordered sites for all atoms except for nonstoichiometric bromine, led ultimately to a highly satisfactory refinement, $R(F^2) = 0.035$, with anisotropic temperature factors and an anisotropic extinction correction.

The derived structure is illustrated in Fig. 1 and the atom positional parameters are given in Table I. The Pt atoms, which are *not crystallographically equivalent*, are almost exactly $c/2$ units apart although not required to be so by symmetry. There is a slight but significant nonplanarity of the $Pt(CN)_4^{-2}$ groups as indicated by the deviation from $z = 0.0$ and 0.5 of the C and N z coordinates. The K^+ ion and H_2O sites are asymmetrically ordered in the cell and are the main source of asymmetry. Finally the surprising discovery was made of what appears to be a low-occupancy Br^- ion site located $0.16c$ from the main Br^- site at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

The most significant structural findings relating to a detailed understanding of the peculiar properties of KCP are probably the information obtained concerning the Pt- and Br-atom distributions. Pt(1) at the origin and Pt(2) with the coordinates $\sim 0\,0\,\frac{1}{2}$ are both completely ordered with small Debye-Waller factors (B is ~0.7 Å^2). The root-mean-square z components of thermal displacement are 0.11 and 0.10 Å, respectively,

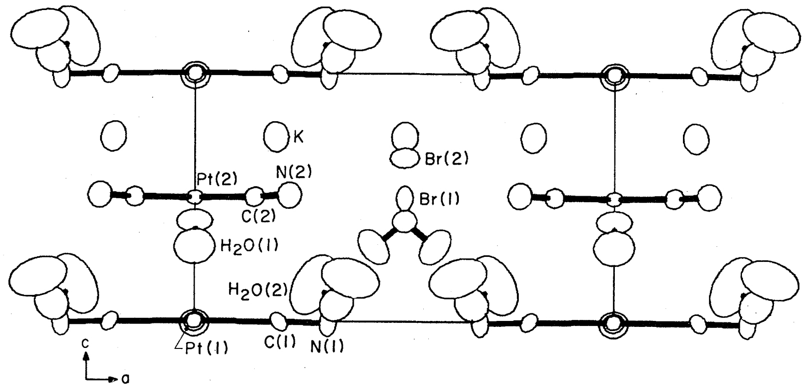

FIG. 1. A b-axis half-cell projection of the structure of $K_2Pt(CN)_4Br_{0.3} \cdot 3H_2O$. Only independent atoms in the asymmetric unit are identified. The Pt atom at the origin is overlapped by C and N atoms. The disordered Br^- sites (separated by $c/6$) are identified as Br(1) and Br(2). Note the asymmetric placement of the K^+ ions and H_2O molecules in the unit cell.

TABLE I. Atom positional parameters for $K_2Pt(CN)_4Br_{0.3} \cdot 3H_2O$.[a,b]

Atom	x	y	z
Pt(1)	0	0	0
Pt(2)	0	0	4997(10)
C(1)	2018(1)	0	− 35(11)
C(2)	1428(1)	1428(1)	5026(8)
N(1)	3183(1)	0	− 96(10)
N(2)	2253(1)	2253(1)	5096(8)
Br(1)[c]	5000	5000	4976(31)
Br(2)[c]	5000	5000	6574(75)
K	1934(4)	5000	7440(14)
O(1)	0	5000	4044(10)
O(2)	3390(4)	3390(4)	696(11)
H(1)	0	4264(6)	3007(14)
H(2)	2843(9)	2843(9)	1443(31)
H(3)	3694(14)	3694(14)	1745(25)

[a] Parameters are multiplied by 10^4.

[b] The estimated standard deviations are given in parentheses and refer to the least-significant figures. Symmetry-fixed coordinates are given without estimates.

[c] The least-squares–derived multipliers for Br(1) and Br(2) are 0.063(3) and 0.023(3). This is equivalent to a total Br content of 0.68 moles per unit cell which in turn suggests that the correct stoichiometry is $K_2Pt(CN)_4Br_{0.34} \cdot 3H_2O$.

which are smaller than the x (y) components (0.12 and 0.13 Å, respectively). These nearly isotropic Pt thermal displacements appear surprising at first glance because of the expectation of charge-density–wave displacements of Pt parallel to c which must be convoluted with the normal thermal displacements. The present results, however, merely place an upper limit on the magnitude of such possible shifts, and small displacements (<0.1 Å) cannot be ruled out.

The existence of two independent bromine sites lined up along c and separated by $c/6$ provides a more complicated anion disorder than previously visualized. The separation of the sites is exactly what is needed to explain the superlattice and accompanying x-ray diffuse scattering observed by Comès *et al.*[5] However such a model fails to give the increase in diffuse intensity with scattering vector which was observed in the x-ray study[5] and which appears to require the sinusoidal displacement associated with a charge-density wave. Thus it is not clear at this stage whether the bromine atoms have important roles in determining the physical properties of KCP as suggested by Inkson[6] or play quite secondary roles. Some doubt about the significance of the second bromine site has been raised by some new measurements on a deuterated crystal of KCP. Although both the H and D data give extra Fourier peaks and least-squares refinements are improved by introduction of bromine at a second site, the thermal parameters associated with the extra sites in the two cases are not in good agreement. Thus the possibility that this site is an artifact due to some type of systematic error has to be entertained.

The structural findings reported here determine a lower symmetry structure and nonequivalent Pt atoms. However this does not imply that we have observed the effects of a static Peierls distortion. Indeed, the dynamic distortion implied by the neutron-inelastic-scattering observation of a Kohn anomaly[7] would appear to be established.

In order to clarify further the possible relationship of the bromine-ion disorder and the properties of this material we are undertaking both low-temperature neutron-diffraction and bromine-quadrupole-resonance studies.

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