

Table 2. Bond distances (Å) and angles (°)

Pt ^{IV} —Br(1)	2.284 (7)	N—Pt—Br(1)	88.5 (5)
Pt ^{IV} —Br(2)	2.684 (6)	Pt—N—C(1)	118 (1)
Pt ^{II} —Br(1)	3.811 (7)	N—C(1)—C(2)	110 (2)
Pt ^{II} —Br(2)	3.411 (6)		
Br(1)—Br(2)	1.127 (9)		
Pt—N	2.09 (1)		
N—C(1)	1.49 (3)		
C(1)—C(2)	1.54 (3)		

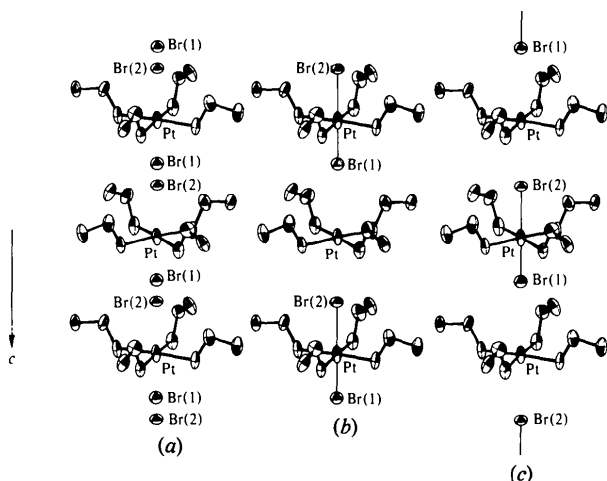


Fig. 1. (a) ORTEP plot (Johnson, 1965) of the chain, rotated 20° around the *a* axis and 40° around the *c* axis. The bromine positions drawn are statistically half-occupied. (b), (c) The same ORTEP plot showing the two possible bromine arrangements along the chain. The bromine positions drawn are fully occupied. (a) is a superposition of (b) and (c).

identical to Fig. 2 of Craven & Hall (1966). Contrary to the results of Craven & Hall (1966), we were able to refine the atomic coordinates with anisotropic temperature factors, and we found it unnecessary to split the Pt position into two half-occupied sites. When we did so, *R* increased to 0.185, and the Br atoms within the chain could not be refined with anisotropic temperature factors.

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Atomic vibrations in the magnesium difluoride crystal. By LINUS PAULING, *Linus Pauling Institute of Science and Medicine, 2700 Sand Hill Road, Menlo Park, California 94025, USA*

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Abstract

The discussion of the anisotropy parameters of the thermal vibrations of the atoms in the magnesium difluoride crystal, as determined by neutron diffraction, is facilitated by

Fig. 1(a) shows the Pt^{II}...Br—Pt^{IV} chain with the two half-occupied Br positions. This figure is quite different from that published earlier (Craven & Hall, 1966; Fig. 1), giving smaller alterations in bond distances along the chain. The differences in Pt^{IV}—Br(1) and Pt^{IV}—Br(2) distances are probably caused by repulsive interactions between Br(2) and the four methylene C atoms [C(1)] of the ligands.

To clarify the problem of one-dimensional order along the chain we have drawn the two possible arrangements of the Br atoms between the Pt atoms (Fig. 1b and c). Fig. 1(a) is the three-dimensional statistical superposition of Figs. 1(b) and 1(c). This finding is very important in interpreting the physical results — especially the resonance Raman data (Clark & Turtle, 1978) for this compound.

As pointed out by Craven & Hall the pattern of continuous diffusive layers and Bragg layers is different in nature from that in other Wolfram's salt analogues. The pattern can be interpreted as follows: The Br atoms along the chains are ordered one-dimensionally but disordered three-dimensionally. All the other atoms of the lattice (ligand atoms, Pt atoms, and Br[−] counterions outside the chains) are ordered three-dimensionally.

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recognizing that each F atom is bonded to the three nearest Mg atoms by a set of coplanar bonds with nearly the same strength, one of the bond lengths being 1.984 Å and the other two 1.994 Å.

Vidal-Valat, Vidal, Zeyen & Kurki-Suonio (1979) have reported values of the thermal-vibration parameters of the atoms in the magnesium difluoride crystal as determined by a neutron-diffraction study at 300 K and 52 K. They conclude from the observed strong anisotropy of the vibration of the F atom at 300 K that there is strong excitation of a libration-like mode of a nearly rigid, linear MgF_2 molecule in the xy plane of the tetragonal crystal. Another way of discussing the observations may, however, have greater significance.

Magnesium difluoride has the rutile structure, with $a = 4.628$, $c = 3.045$ Å, and the oxygen parameter $x = 0.3032$. With these values the linear F–Mg–F group has bond lengths of 1.984 Å, as stated by Vidal-Valat *et al.* (1979). The value of x , however, is close to $[(c/a)^2 + 2]/8 = 0.3041$, which places six atoms at the same distance from the Mg atom (Pauling, 1928); in fact, with $x = 0.3032$ there are four F atoms with Mg–F bond lengths of 1.994 Å, only 0.5% greater than for the other two.

It is accordingly not justified to describe the crystal as containing linear F–Mg–F molecules. Instead, it has a framework structure, with each Mg atom forming six bonds with F atoms at the corners of a somewhat distorted octa-

hedron (two opposite edges, shared between octahedra, shortened to 2.576 Å) and each F atom forming three bonds in a vertical plane, with bond angles 99.5, 130.2, 130.2°. All vibrations of atoms relative to their neighbors would thus involve a change in length of strong bonds except the vibration of the F atom perpendicular to the plane of its three bonds. The values of the mean-square principal amplitudes of vibration given by Vidal-Valat *et al.* (1979) (averages of seven values corresponding to different assumptions about extinction) are the following, in order U_{33} (along the c axis), U_{11} , and U_{11} , all in units 10^{-4} Å; at 52 K, 13, 19, 14 for Mg and 23, 31, 40 for F; and at 300 K, 31, 42, 52 for Mg and 56, 49, 115 for F. As pointed out by Vidal-Valat *et al.* (1979), the strikingly large amplitude is that of the F atom at 300 K; also it is in the direction that does not involve first-order stretching and compression of Mg–F bonds.

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Change of publisher of *Structure Reports, Molecular Structures and Dimensions* and other publications

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Notes and News

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Proceedings of the International Symposium on Biomolecular Structure, Conformation, Function & Evolution held at Madras in January 1978

These proceedings, covering over a hundred articles presented

at the above Symposium, are being published by Pergamon Press in two volumes edited by Professor R. Srinivasan and others. The volumes are expected to be available in early 1980. Vol. I might be of interest to crystallographers as it deals with 'Diffraction and Related Studies' on biomolecules.