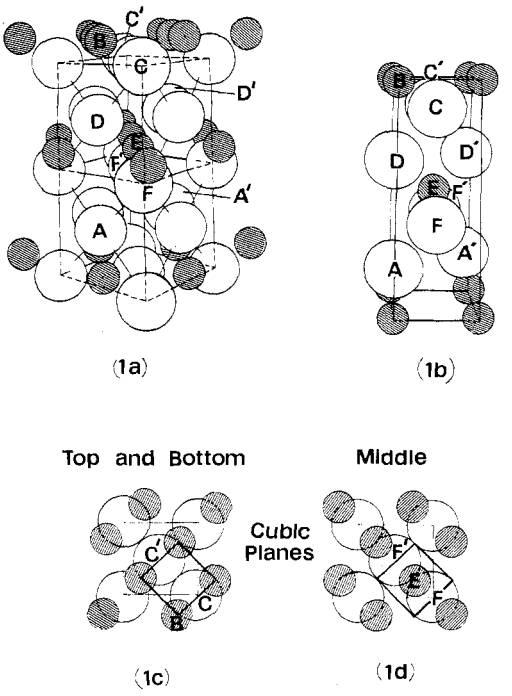

Figure 1. (a) Face-centered cubic iodide lattice. (b) Mercuric iodide unit cell. (c and d) Partial projective sections of planes of (a) and (b), the cubic unit cell being shown faint and the mercuric iodide unit cell bold. In this figure all atoms have been labeled in a similar manner to those of Figure 2 of ref 3.

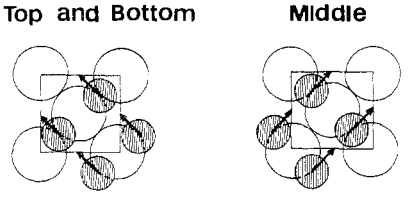

Figure 2. Displacement of mercury atoms from their positions shown in Figure 1b and c. All displacements are $a/2(2^{1/2})$.

the correct factor group representations (Table I) would then require that all the vibrating modes which have gerade characteristics in Table I correlate with acoustic modes in the D_{4h}^1 factor group. It follows that, on this model, all Raman-active modes of HgI_2 would be expected to have frequencies much lower than the infrared-active modes. This

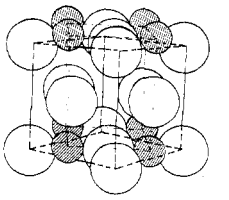

Figure 3. Unit cell of D_{4h}^1 symmetry generated by the displacements indicated in Figure 2.

is not in accord with the spectral observations. We conclude that the interpretation of the vibrational spectra of HgI_2 cannot be aided by recourse to a D_{4h}^1 factor group.

There are several cubic AB_2 lattices in which the B atoms are cubic close packed and the A atoms are distributed over appropriate holes. Cuprite, Cu_2O, is one example. Anatate, TiO_2, with the tetragonal distortion removed, is another. However, their unit cells each require several AB_2 molecules in a unit cell and so do not provide a basis for a simple explanation of the vibrational spectra of HgI_2.

We conclude that there seems to be no reason for discussing the vibrational spectrum of HgI_2 in any factor group other than D_{4h}^{15}.

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Registry No. HgI_2, 7774-29-0.

References and Notes

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Additions and Corrections

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Robert C. Pierce and Richard F. Porter*: Ion–Molecule Chemistry of BF_3 and HBF_2 in Hydrogen.

Pages 1087–1092. All third-order rate constants (k_3) appearing in Table III and in the text should have the units $cm^6/(molecule^2\ sec)$.