

The idealized picture of a perfect ionic crystal would involve a valence band constructed entirely from anion wave functions and a conduction band made entirely from cation wave functions. Since one would anticipate a much larger deformation of the conduction band than of the valence band with pressure, one would expect the pressure effect to be independent of the anion for lattices with the same band structure. ¹Figure 6(10) shows the shift of the edge for three compounds having the structure O_h , and for two compounds having the structure V_h ¹⁶, and one finds that the assumption is quite good.

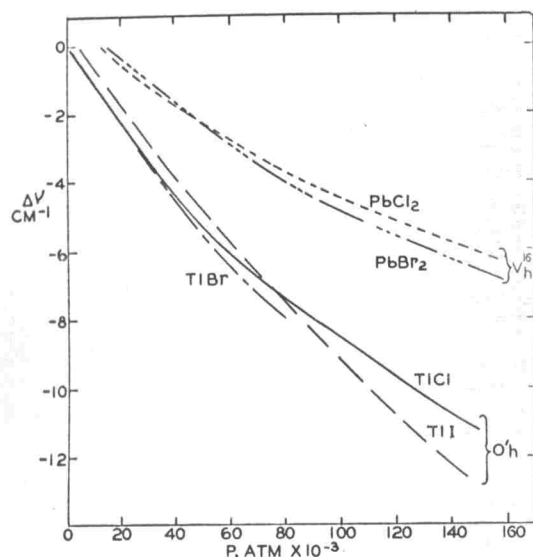


Fig. 6 Shift of absorption edge with pressure-ionic crystals.

On the other hand, a typical molecular crystal shows a good deal of sharing of wave functions in both the valence and conduction bands. Figure 7⁽¹¹⁾ shows that in this case the shift is quite dependent on the more electronegative atom.

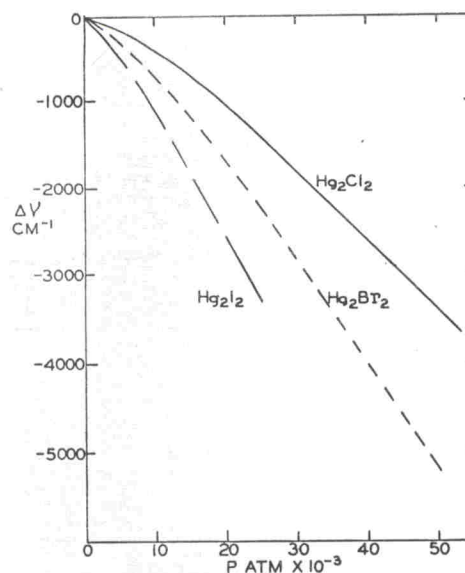


Fig. 7 Shift of absorption edge with pressure-molecular crystals.