The high pressure orthorhombic patterns were given an approximate indexing by a computer program for indexing X ray diffraction patterns written at Battelle Northwest (28) and adapted for use on the IBM 7040 by Alan Webb. This program applies the analytical procedure discussed by Azaroff and Buerger (29) in which Miller indicies are assigned to the observed d values by systematic trial and error until a set of indicies can be found which give consistent lattice parameters. For the isometric systems the relation

$$d^2_{hkl} = \frac{a^2}{h^2 + k^2 + l^2} \qquad (1)$$

was used and for the orthorhombic systems the relation

$$\frac{1}{d^2_{hkl}} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \qquad (2)$$

was used. In these relations d = interplanar spacing, h,k,l = Miller indicies, and a,b,c = lattice parameters. When the hkl values are successfully assigned to the observed d values so that the lattice parameters calculated from all observed d values are consistent the pattern is said to be indexed.

The high pressure orthorhombic patterns could not be indexed to cubic, hexagonal or tetragonal structures with the above method but several different orthorhombic indexings were possible.

The orthorhombic indexing giving closest to two molecules per unit cell was chosen and refined by trial and