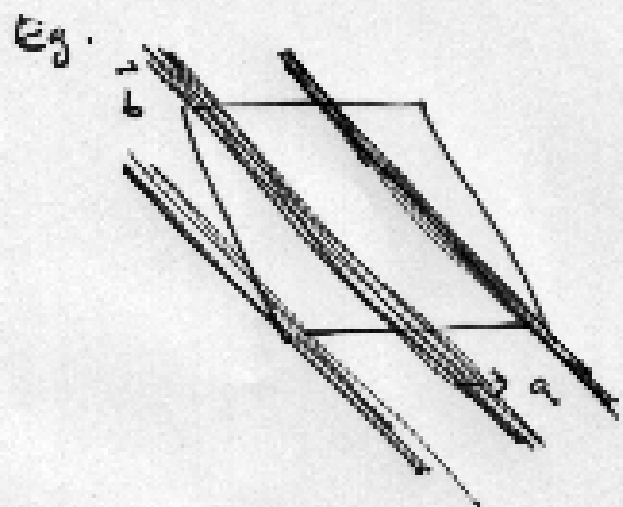


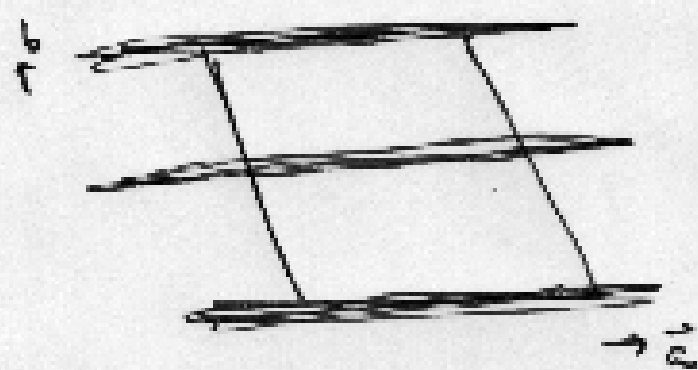
# Supplement

1. We have seen that the plane waves we are interested in are plane waves which intersect the corner of the unit cells.

The Miller construction tells us to count the number of times the plane wave crosses the axes.



is the  $(2\ 1\ 0)$  plane or reflection

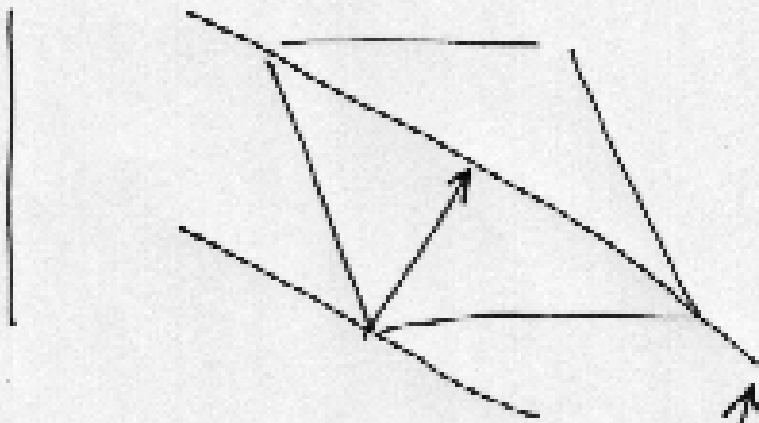


When the plane is // to an axis direction the index for the direction is 0.

$\therefore (0\ 2\ 0)$  plane or reflection.

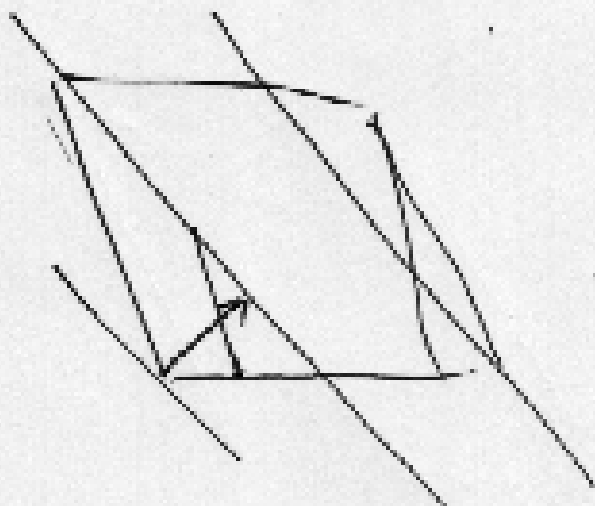
2. We now wish to come up with mathematical formulas for these plane waves.

All plane waves can be described as 
$$e^{2\pi i \vec{k} \cdot \vec{r}}$$
 where  $\vec{r}$  is the spatial coordinate.



$$(a^* + b^*)$$

$$x a + (1-x) b$$



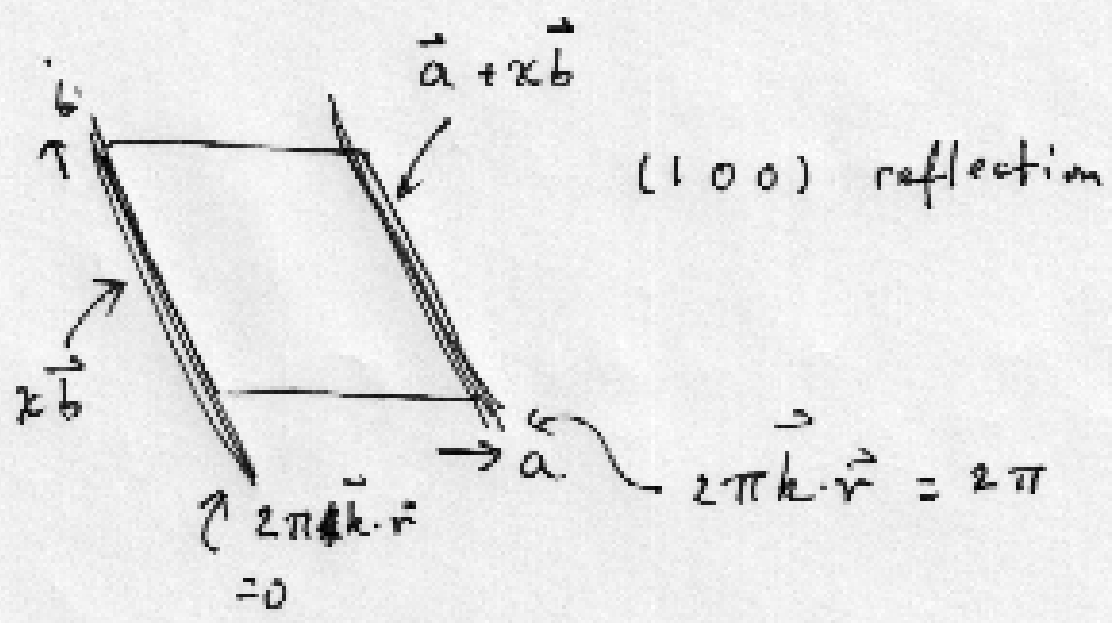
$$(2 \ 1 \ 0)$$

$$2x \vec{b} + \left(\frac{1}{2} - x\right) \vec{a}$$

$$\frac{1}{2}, \frac{1}{4}$$

$$-2x \vec{a} + 2x \vec{b} + 1$$

3.



$$\vec{k} \cdot x\vec{b} = 0 \quad \therefore \vec{k} \perp \vec{b}$$

$$(a + x\vec{b}) \cdot \vec{k} = 1$$

$$\therefore \vec{k} \cdot \vec{a} = 1$$

$$(100) = 1a^*$$

$$a^* \perp \vec{b}$$

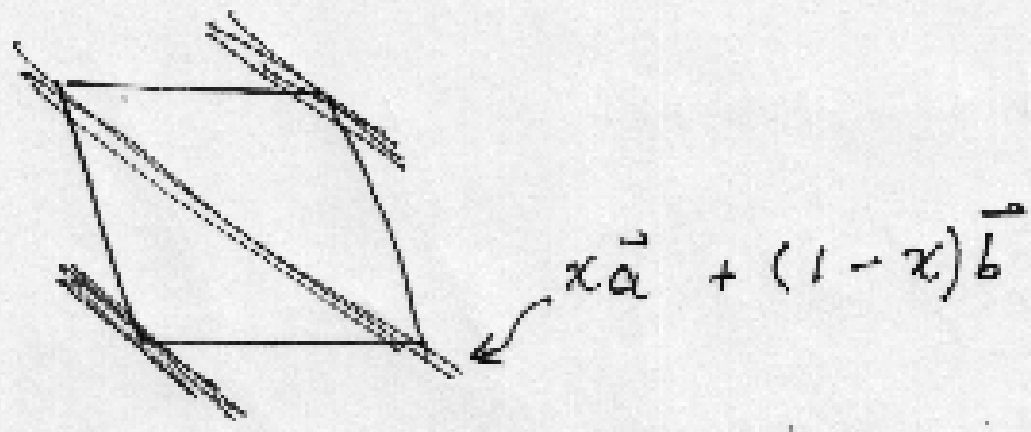
$$a^* \cdot \vec{a} = 1$$

Same applies for  $\vec{b}^*$  (010)

$$\vec{b}^* \perp \vec{a}$$

$$b^* \cdot \vec{b} = 1$$

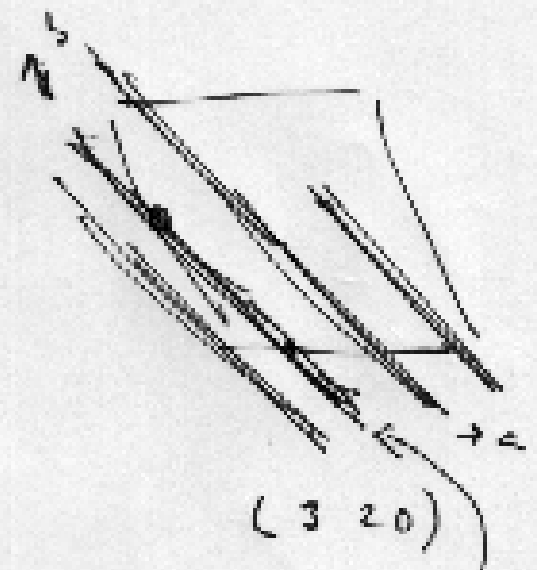
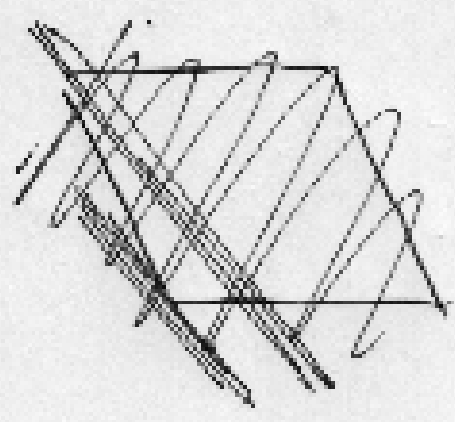
4.



Note  $(1 \ 1 \ 0) = 1 \vec{a} + 1 \vec{b}$

$$(\vec{a} + \vec{b}) \cdot (x\vec{a} + (1-x)\vec{b}) = 1$$

5. Consider



$$\left(\frac{1}{3}\right)\vec{a} + \left(\frac{2}{2}\right)\vec{b}$$

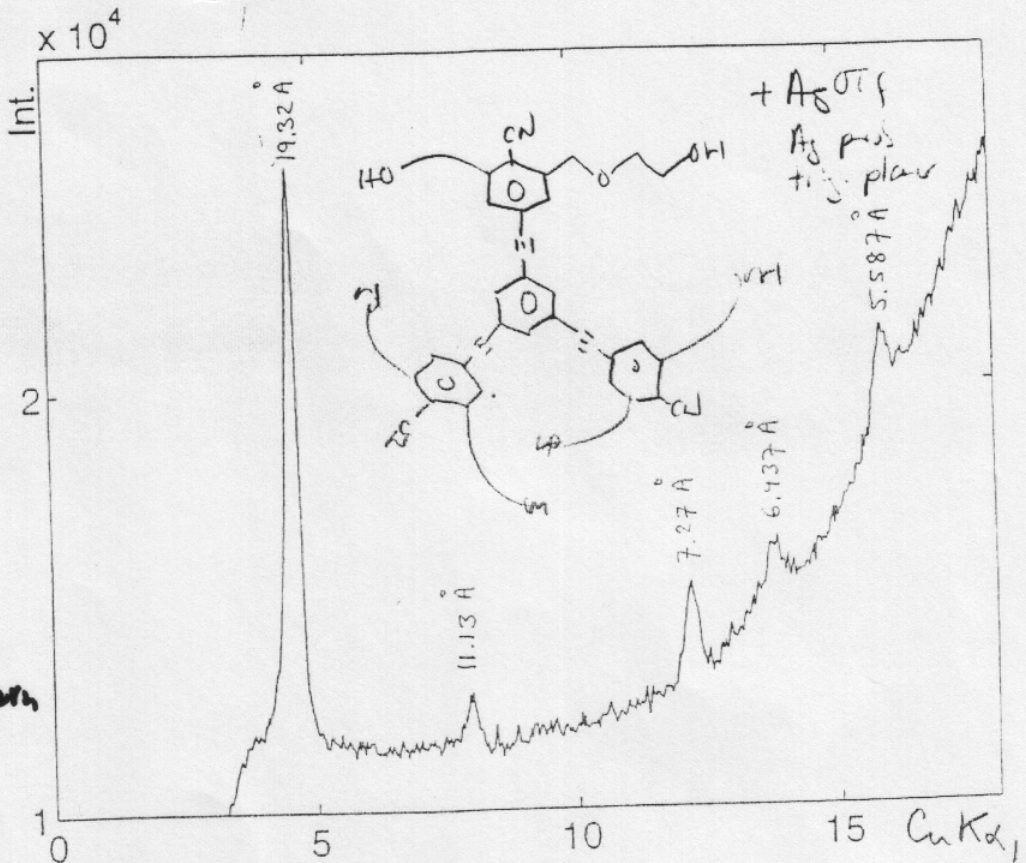
$$(3 \ 2 \ 0) = 3\vec{a} + 2\vec{b}$$

$$(h \ k \ l) = h\vec{a} + k\vec{b} + l\vec{c}$$

where  $h, k$  &  $l$  are integers.

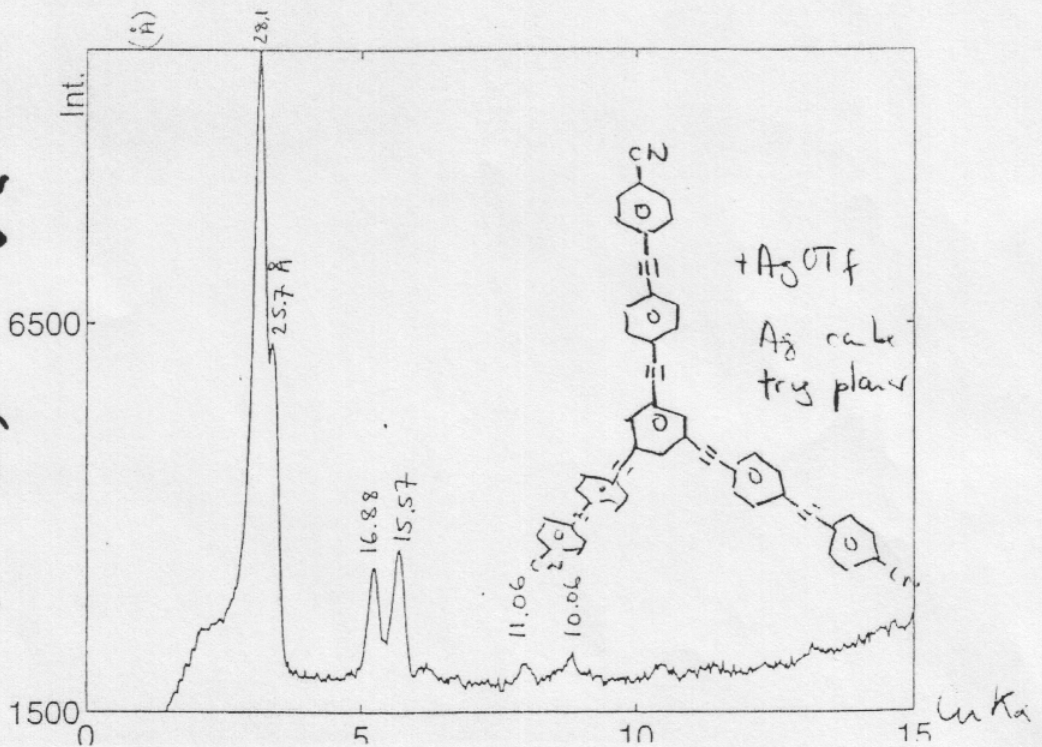
# Problem Set 2

1.  
Find the 2-dim. unit cell axes & the names of the planes (diffraction planes) for this → powder pattern



2.  
Same as 1 for this powder pattern →

[useful data on attached sheets]



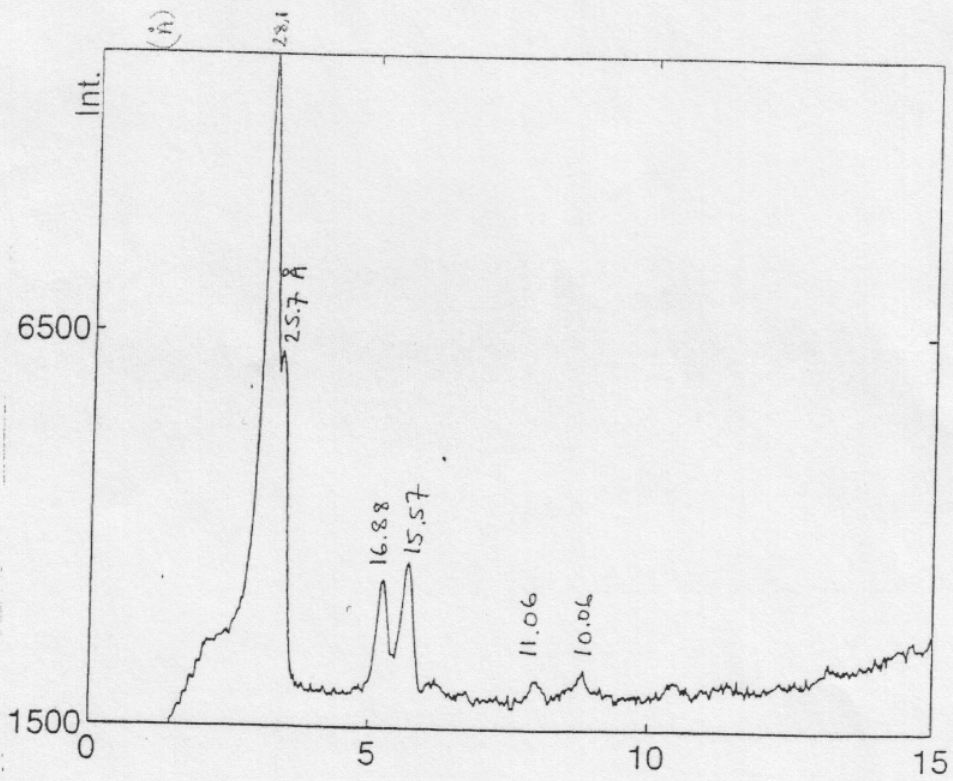
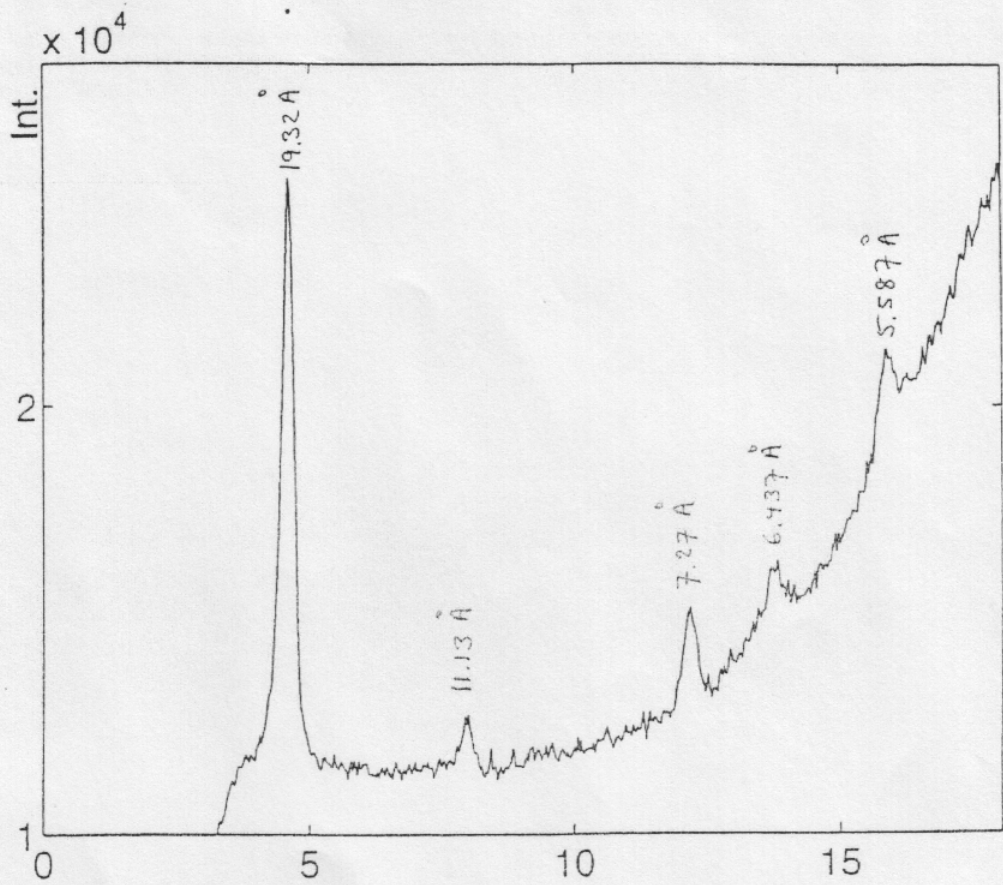




TABLE 2.4. Expressions for  $d^*(hkl)$  and  $d(hkl)$  in the Seven Crystal Systems<sup>a</sup>

System	$d^*(hkl)$	$d^2(hkl)$	$d^2(hkl)$
Triclinic	$h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2klb^*c^* \cos \alpha^*$ $+ 2lhc^*a^* \cos \beta^* + 2hka^*b^* \cos \gamma^*$	$K^2/d^{*2}(hkl)$	$d^2(hkl)$
Monoclinic	$h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2hla^*c^* \cos \beta^*$	$\left\{ \frac{1}{\sin^2 \beta} \left[ \frac{h^2}{a^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right] + \frac{k^2}{b^2} \right\}^{-1}$	
Orthorhombic	$h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2}$	$\left\{ \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right\}^{-1}$	
Tetragonal	$(h^2 + k^2)a^{*2} + l^2 c^{*2}$	$\left\{ \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2} \right\}^{-1}$	
Hexagonal and trigonal (P)	$(h^2 + k^2 + hk)a^{*2} + l^2 c^{*2}$	$\left\{ \frac{4(h^2 + k^2 + hk)}{3a^2} + \frac{l^2}{c^2} \right\}^{-1}$	
Trigonal (R) (rhombohedral)	$[h^2 + k^2 + l^2 + 2(hk + kl + hl)(\cos \alpha^*)]a^{*2}$	$a^2(TR)^{-1}$ , where $T = h^2 + k^2 + l^2 + 2(hk + kl + hl)(\cos^2 \alpha - \cos \alpha) / \sin^2 \alpha$ and $R = (\sin^2 \alpha) / (1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha)$	
Cubic	$(h^2 + k^2 + l^2)a^{*2}$	$\left\{ \frac{h^2 + k^2 + l^2}{a^2} \right\}^{-1} = \frac{a^2}{h^2 + k^2 + l^2}$	

<sup>a</sup> In the monoclinic system,  $d(100) = a \sin \beta$ ,  $d(001) = c \sin \beta$ , and hence  $a = K/(a^* \sin \beta^*)$  and  $c = K/(c^* \sin \beta^*)$ .

In the hexagonal system (and trigonal P),  $a = b = K/(a^* \sin \gamma^*) = K/(a^* \sqrt{3}/2)$ .

In general, the expressions for  $d^{*2}$  are simpler in form than the corresponding expressions for  $d^2$ .

**TABLE 1.5** Bond distances  
*The values given are average lengths and do not necessarily apply exactly to the compounds mentioned<sup>62</sup>*

Bond type	Length, Å	Typical compounds		
<b>C—C</b>				
$sp^3-sp^3$	1.53			
$sp^3-sp^2$	1.51	Acetaldehyde, toluene, propene		
$sp^3-sp$	1.47	Acetonitrile, propyne		
$sp^2-sp^2$	1.48	Butadiene, glyoxal, biphenyl		
$sp^2-sp$	1.43	Acrylonitrile, vinylacetylene		
$sp-sp$	1.38	Cyanoacetylene, butadiyne		
<b>C=C</b>				
$sp^2-sp^2$	1.32	Ethylene		
$sp^2-sp$	1.31	Ketene, allenes		
$sp-sp^{63}$	1.28	Butatriene, carbon suboxide		
<b>C≡C<sup>64</sup></b>				
$sp-sp$	1.18	Acetylene		
<b>C—H<sup>65</sup></b>				
$sp^3-H$	1.09	Methane		
$sp^2-H$	1.08	Benzene, ethylene		
$sp-H^{66}$	1.08	HCN, acetylene		
<b>C—O</b>				
$sp^3-O$	1.43	Dimethyl ether, ethanol		
$sp^2-O$	1.34	Formic acid		
<b>C=O</b>				
$sp^2-O$	1.21	Formaldehyde, formic acid		
$sp-O^{57}$	1.16	CO <sub>2</sub>		
<b>C—N</b>				
$sp^3-N$	1.47	Methylamine		
$sp^2-N$	1.38	Formamide		
<b>C=N</b>				
$sp^2-N$	1.28	Oximes, imines		
<b>C≡N</b>				
$sp-N$	1.14	HCN		
<b>C—S</b>				
$sp^3-S$	1.82	Methanethiol		
$sp^2-S$	1.75	Diphenyl sulfide		
$sp-S$	1.68	CH <sub>3</sub> SCN		
<b>C=S</b>				
$sp-S$	1.67	CS <sub>2</sub>		
<b>C—halogen<sup>67</sup></b>		<b>F</b> <b>Cl</b> <b>Br</b> <b>I</b>		
$sp^3-halogen$	1.40	1.79	1.97	2.16
$sp^2-halogen$	1.34	1.73	1.88	2.10
$sp-halogen$	1.27 <sup>68</sup>	1.63	1.79 <sup>69</sup>	1.99 <sup>69</sup>

**Ag—N**      **~2.2 Å**

<sup>62</sup>For an accurate method of C—H bond distance determination, see Henry *Acc. Chem. Res.* **1987**, *20*, 429-4.

<sup>63</sup>Bartell; Roth; Hollowell; Kuchitsu; Young *J. Chem. Phys.* **1965**, *42*, 2683.

<sup>64</sup>For reviews of carbon-halogen bonds, see Trotter, in Patai *The Chemistry of the Carbon-Halogen Bond*, pt Wiley: New York, 1973, pp. 49-62; Mikhailov *Russ. Chem. Rev.* **1971**, *40*, 983-997.

<sup>65</sup>Lide, *Tetrahedron* **1962**, *17*, 125.

<sup>66</sup>Rajput; Chandra *Bull. Chem. Soc. Jpn.* **1966**, *39*, 1854.

<sup>67</sup>Schwendeman; Tobiason *J. Chem. Phys.* **1965**, *43*, 201.

<sup>68</sup>For a review of this concept, see Bingel; Lüttke *Angew. Chem. Int. Ed. Engl.* **1981**, *20*, 899-910 [*Angew. Ch.* **93**, 944-956].