7. Direct Methods

Problems

7.1. The measurement of diffracted intensities reveals the moduli of the structure factors, but not the signs. For a particular monatomic, 1-D crystal, the structure factors F_h are related by:

$$6S_h|F_h| = \sum_{h'=0}^{5} S_{h'}S_{h-h'}|F_{h'}F_{h-h'}|$$

where $S_h = \pm 1$. This gives the five equations below:

i) $6S_1 = 8S_1 + S_1S_2 + 2S_2S_3 + 2S_3S_4 + S_4S_5$

ii) $6S_2 = 8S_2 + 1 + 2S_1S_3 + S_2S_4 + 2S_3S_5$

iii) $12S_3 = 16S_3 + 2S_1S_2 + S_1S_4 + S_2S_5$

iv) $6S_4 = 8S_4 + 4S_1S_3 + 1 + S_1S_5$

v) $6S_5 = 8S_5 + 2S_1S_4 + 4S_2S_3$

If we know $S_1 = +1$, determine the remaining signs S_2 through S_5 that satisfy these equations.

7.2. The magnitudes of the normalized structure factors E_h for the first 21 Fourier components from a centrosymmetric, 1-D crystal with five point-like atoms are listed below:

h	$\|E_h\|$		h	$\|E_h\|$
0	1.0000			
1	0.5011		11	0.2932
2	0.6469		12	0.2253
3	0.0550		13	0.8701
4	0.1197		14	0.5380
5	0.3453		15	0.8155
6	0.1560		16	0.1717
7	0.0504		17	0.3254
8	0.5167		18	0.2094
9	0.1491		19	0.2242
10	0.4000		20	0.0000

a) At least two E_h values can be proven to be positive. Find which ones they are. (Hint: Some may have $h > 20$.)

b) Additional data show that $S_{13} = +1$. Determine the value of S_{15}.

c) Further experiments confirm that $S_1 = -1$. Determine the value of S_{14}.