NOTE 1: Recipe to resolve structure from a diffraction experiment.

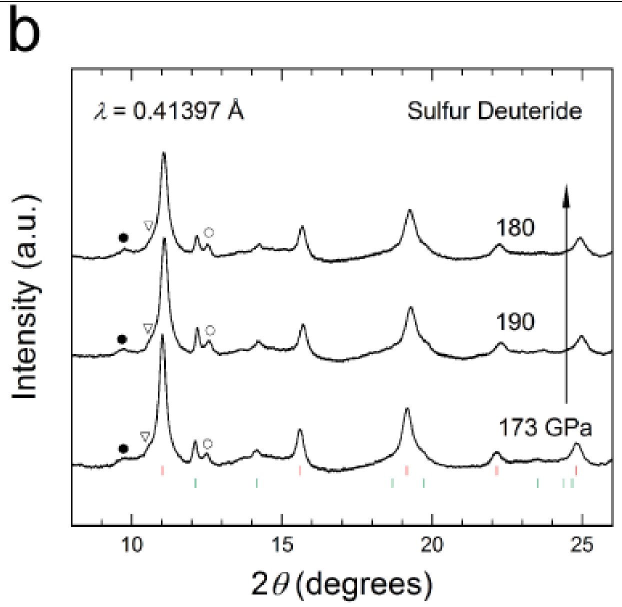

Figure 1.
This is the x-ray diffraction data taken on new high temperature Sulfur Deuteride superconductor [see *Nature* **525**, 73–76 (2015)]. At ambient pressure this material is a toxic gas that crystalize under high pressure. The pressure conditions of this experiment are indicated in the figure that shows diffracted intensity versus scattering angle 2θ.
This figure is taken from http://arxiv.org/abs/1509.03156

TASK:
What crystal structure does Sulfur Deuteride have under high pressure?

STEP 1: Complete table 1

Table 1: The plane distance d = $2\pi/\sqrt{h^2+k^2+l^2}$ for different Miller indices (hkl) and the structure factor S for different structures.

Index i	(hkl)	d (2π)	Structure Factor S_{BCC}	S_{FCC}	$S_{DIAMOND}$
1	(100)	1	= 0		
2	(110)	$1/\sqrt{2}$	$\neq 0$		
3	(111)	$1/\sqrt{3}$	= 0		
4	(200)	$1/2$	$\neq 0$		
5	(210)	$1/5$	= 0		
6	(211)	$1/\sqrt{6}$	$\neq 0$		
7	(220)	$1/\sqrt{8}$	$\neq 0$		
8	(221)	$1/3$	= 0		
9	(300)	$1/3$	= 0		
10	(310)	$1/\sqrt{10}$	$\neq 0$		
11	(311)	$1/\sqrt{11}$	= 0		
12	(400)	$1/4$	$\neq 0$		

STEP 2: Consider Bragg's Law - $n\lambda = 2d\,sin(\theta)$ - where n is an integer, λ is the x-ray wave length and d is the plane distance and 2θ is the scattering angle. Now since $n\lambda$ is the same for all the peaks measured, we have

$$\frac{d(1)}{d(PN)} = \frac{\sin\,[\theta(PN)]}{\sin[\theta(1)]}$$

where PN means “Peak Number”. The first peak (from left) in Fig. 1 has PN= 1 and so forth. Now we can read-off the peak positions (in 2θ) of the peaks indicated by small read bars.

Table 2: Column with PN and 2θ is derived from Figure 1. Column 3 is derived from column 2. The ratios d(1) / d(PN) [BCC] and d(1) / d(PN) [FCC] can be derived from Table 1.

Peak Number (PN)	2θ (Degrees)	$\frac{\mathrm{Sin}[\theta(\mathrm{PN})]}{\mathrm{Sin}[\theta\ (\mathrm{PN}=1)]}$	$\frac{d(1)}{d(PN)}[BCC]$	$\frac{d(1)}{d(PN)}[FCC]$
1	11	1	1	
2	15.7	1.4	$\sqrt{2}$	
3	19.2	1.7	$\sqrt{3}$	
4	22.1	2	2	
5	24.9	2.25	$\sqrt{10}$	

Conclusion: The BCC structure explains quite well the observed data. One should however exclude that other structures (for example FCC and diamond-structure) are not providing and equally good agreement.