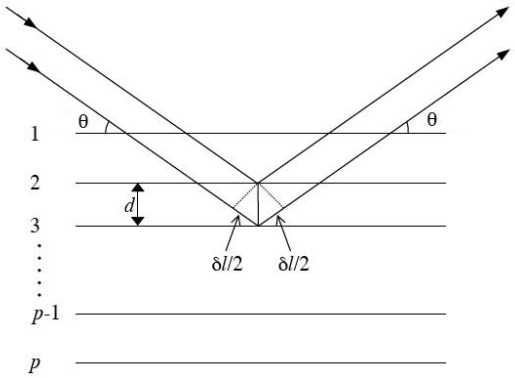
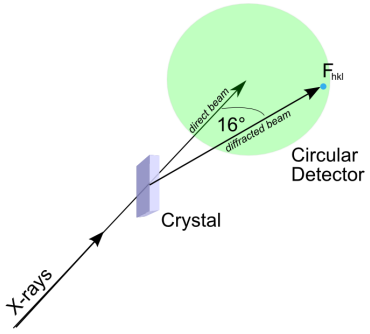
BC530 2014 X-ray Crystallography Unit Homework

Bragg's Law and measured Bragg relections

The Bragg planes for a reflection [h k l] and another reflection [2h 2k 2l] are parallel. Therefore the same diagram showing the conditions for satisfying the Bragg diffraction condition can be used to show the values of λ, d , and θ required for both reflections.





1. Sketch on the diagram above what is different about diffraction of the [h k l] and [2h 2k 2l] relections.
2. Does this mean that the amplitudes ($|F| = amplitude = \sqrt{intensity}$) measured experimentally for the two reflections are the same? I.e. is it true that $|F_{hkl}| = |F_{2h2k2l}|$? Why or why not?
3. Where do the [h k l] and [2h 2k 2l] "spots" appear on the recorded diffraction image (right figure)?

Evaluate Structures from a Recent Report

Here is the Supplementary Table 1 (to which I have added a few lines) from a recent structure determination of the c-di-AMP riboswitch, an RNA mediator of a bacterial signalling pathway related to DNA damage [*Gao & Serganov, Nature Chemical Biology 10, 787–792 (2014) doi:10.1038/nchembio.1607*].

Supplementary Table 1 Data collection, phasing and refinement statistics

	T. pseudethanolicus $[Ir(NH_3)_6]^{3+}$-soaked	*T. pseudethanolicus* Native	*T. lienii* Native
PDB Entry Code	**4QKA**	**4QK8**	**4QK9**
X-ray source			
synchrotron	NSLS X25	APS 24-ID	NSLS X25
wavelength	1.105Å	0.9792Å	1.105Å
Data collection			
Space group	$P3_121$	$P3_121$	$P2_13$
Cell dimensions			
a, *b*, *c* (Å)	116.0, 116.0, 114.1	114.9, 114.9, 114.7	110.3, 110.3, 110.3
α, *β*, *γ* (°)	90.0, 90.0, 120.0	90.0, 90.0, 120.0	90.0, 90.0, 90.0
Resolution (Å)	30.00-3.20 (3.31-3.20) *	30.00-3.05 (3.16-3.05)	30.00-3.00 (3.11-3.00)
R_{sym} or R_{merge}	0.12 (0.71)	0.07 (0.52)	0.11 (0.55)
$I/\sigma I$	37.3 (3.0)	34.7 (3.5)	40.4 (6.0)
Completeness (%)	100.0 (99.7)	99.6 (99.9)	99.8 (100.0)
Redundancy	17.7 (12.1)	6.0 (6.1)	11.5 (12.2)
Refinement			
Resolution (Å)	30.00-3.20	30.00-3.05	30.00-3.00
No. reflections	28,200	16,997	9,173
R_{work}/ R_{free}	17.1 / 19.7	18.1 / 19.5	18.2 / 22.4
No. atoms			
RNA	2,578	2,626	2,516
Ligand/ion	130	98	99
Water	2	4	0
B-factors			
RNA	99.4	90.9	57.2
Ligand/ion	84.9	63.0	43.3
Water	56.7	56.1	----
R.m.s deviations			
Bond lengths (Å)	1.049	1.051	0.987
Bond angles (°)	0.005	0.005	0.005

*Highest resolution shell is shown in parenthesis.

1. What is the resolution of the structure? Why are there two lines in the table marked "Resolution"?

2. When you collect data at a synchrotron you can choose what wavelength X-rays are used. Why do you suppose they chose one wavelength for the data collected at NSLS and a different wavelength for the data collected at APS?

3. What indications do you have that this sructure determination and refinement was done well, or poorly?

4. I said in class that the Ramachandran chart is one of the few quality checks you can expect to see in a good crystal structure report, but there is no indication of Ramachandran chart quality in this table. Should we fault them for this lack? You can find equivalent information on the PDB web site for these three structures. Is the quality good or bad?
   http://www.pdb.org/pdb/explore/explore.do?structureId=4QK8

5. Just considering the information in the Table 1, how do you think they solved these structure? That is, how might they have gotten initial phases to calculate electron density maps into which they could build and refine structural models?