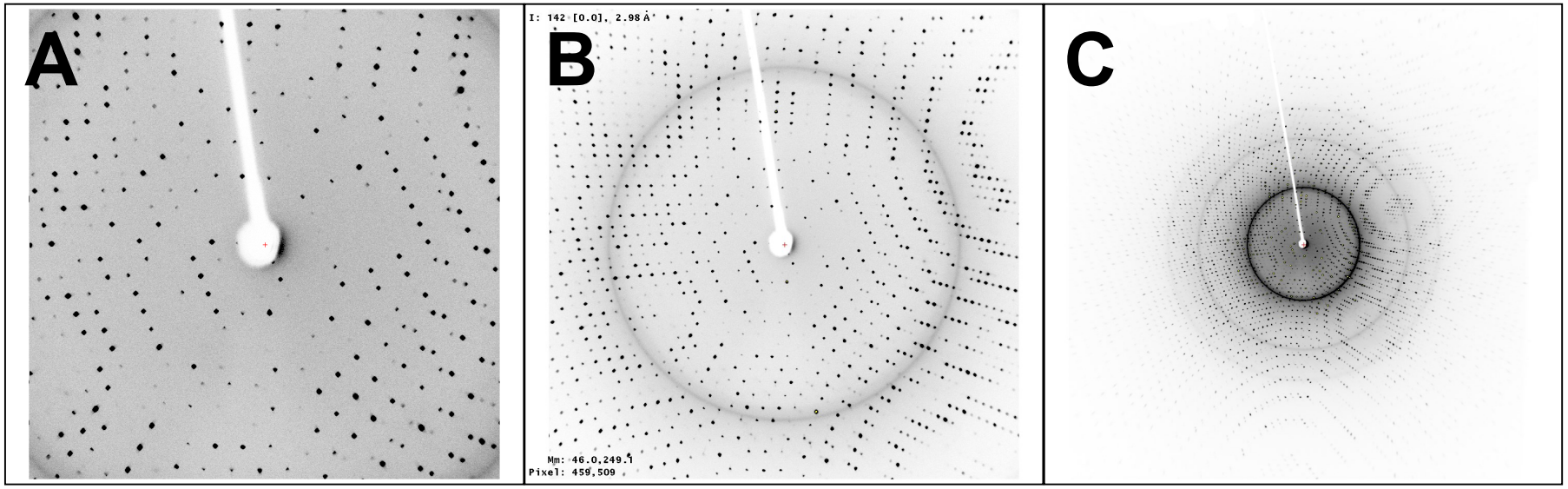
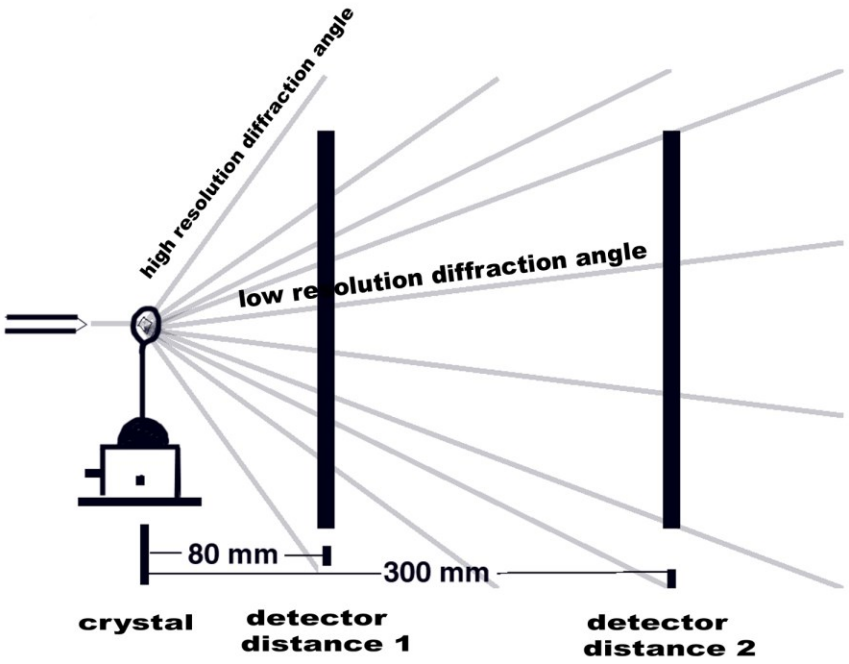
Distance

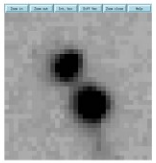
The 3 diffraction images below were recorded using different crystal-to-detector distances. Match each image with its corresponding distance: 80, 250, or 450 mm. All patterns were recorded from the same crystal using the same X-ray wavelength.

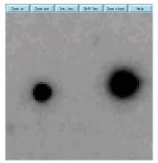


_____ _____ _____

DISTANCE







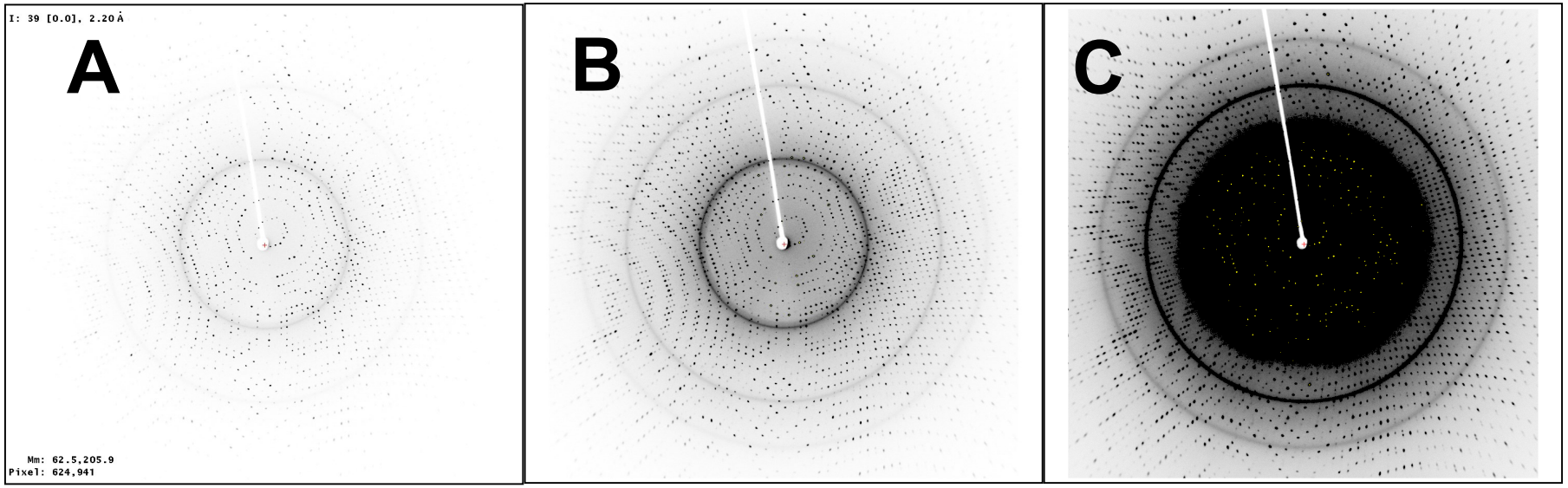
short distance — **long distance**

+able to collect high angle (resolution) diffraction
-danger of operlapping spots on detector
(i.e. poor spatial resolution)
practical when the unit cell is small (<100 Ang)
60 mm minimum distance

limited to low angle (resolution) diffraction -
no danger of overlapping spots on detector +
(i.e. good spatial resolution)
necessary when unit cell is large (>100 Ang)
350 mm maximum distance

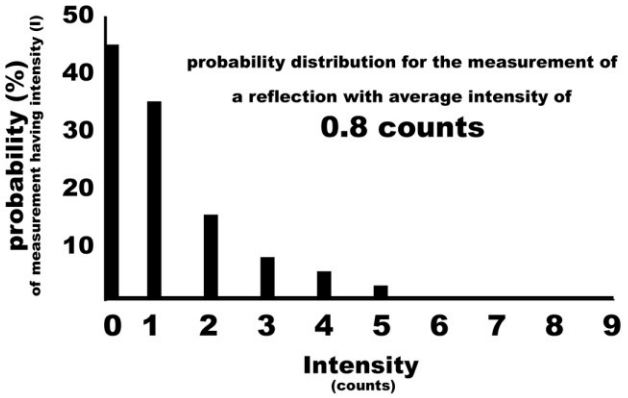
Time

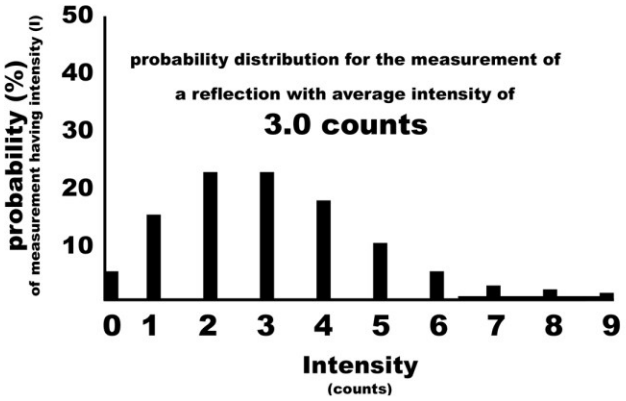
The 3 diffraction images below were recorded using exposure times. Match each image with its corresponding length of exposure: 12 s, 60 s, or 300 s. All patterns were recorded from the same crystal using the same X-ray wavelength.



_____ _____ _____

TIME





for Poisson distribution

$$\sigma_I = \sqrt{\bar{I}}$$

$$\text{fractional uncertainty} = \frac{\sigma_I}{\bar{I}} = \frac{\sqrt{\bar{I}}}{\bar{I}} = \frac{1}{\sqrt{\bar{I}}}$$

fractional uncertainty = $\frac{1}{\sqrt{0.8}}$ =1.118

smaller σ, but larger fractional uncertainty

fractional uncertainty = $\frac{1}{\sqrt{3}}$ = 0.577

lager σ, but smaller fractional uncertainty

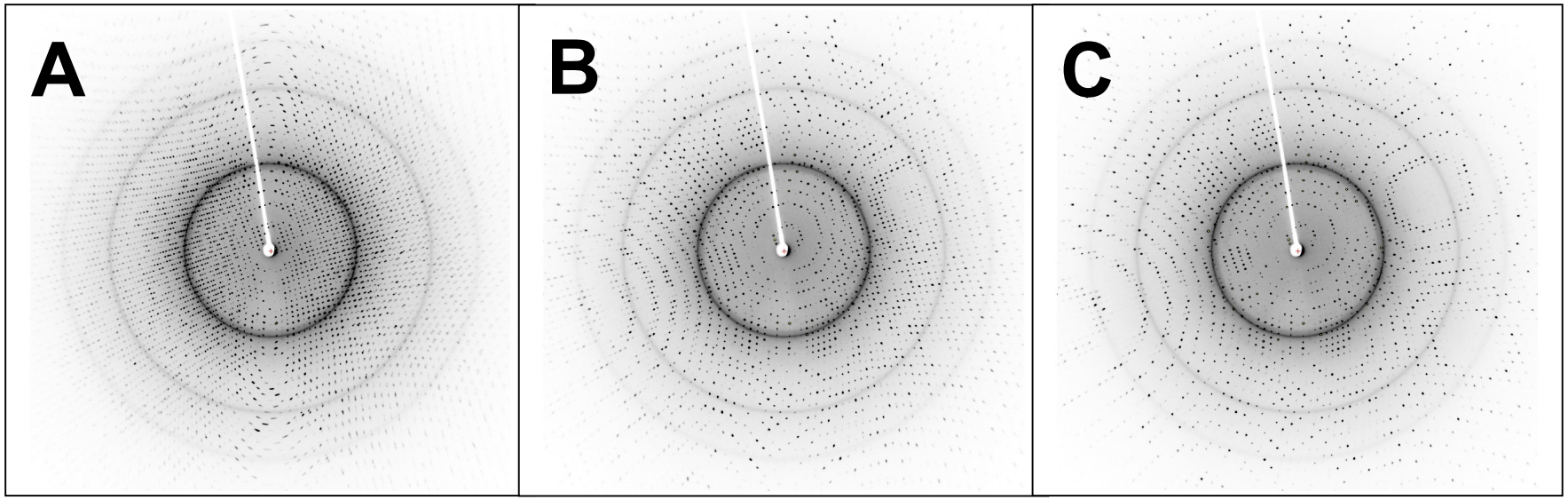
short exposure — **long exposure**

+ quicker data set
- less accurate measurements
+ no chance of overloading detector pixels
practical for big crystals
or high intensity synchrotron beams.
1 sec/exposure at synchrotron

time consuming -
more accurate measurements +
may overload detector pixels -
necessary for small crystals
or weaker home x-ray sources
3 min/exposure on CCD home source

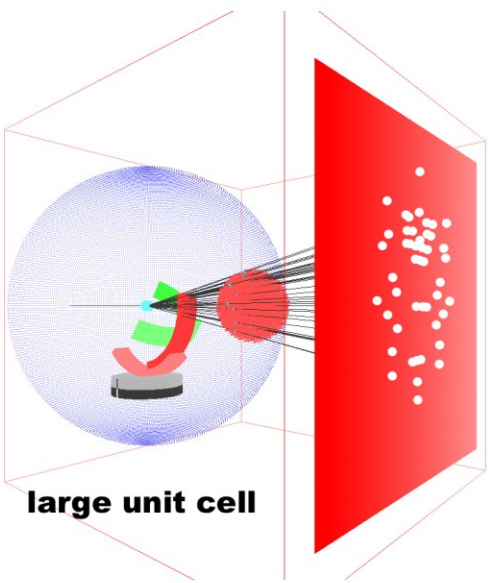
Oscillation Angle

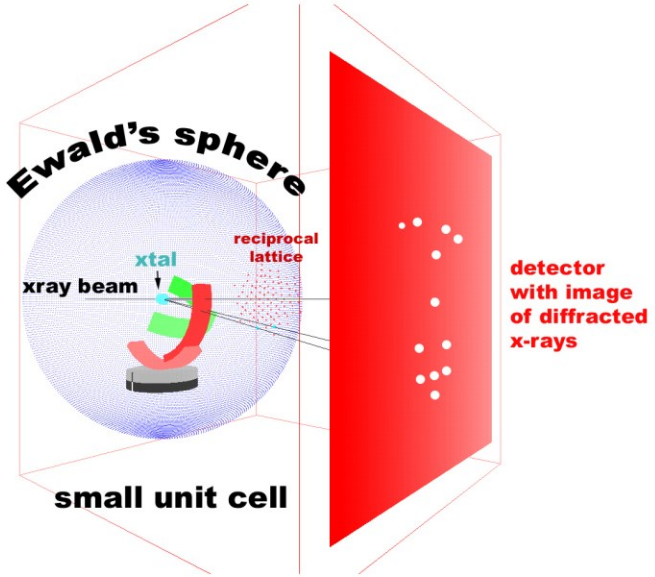
The 3 diffraction images below were recorded while rotating the crystal by different amounts. Match each image with its corresponding rotation: 0.10°, 1.00°, or 5.00°. All images were recorded from the same crystal at the same X-ray wavelength.



_____ _____ _____

OSCILLATION ANGLE





fewer degrees oscillation

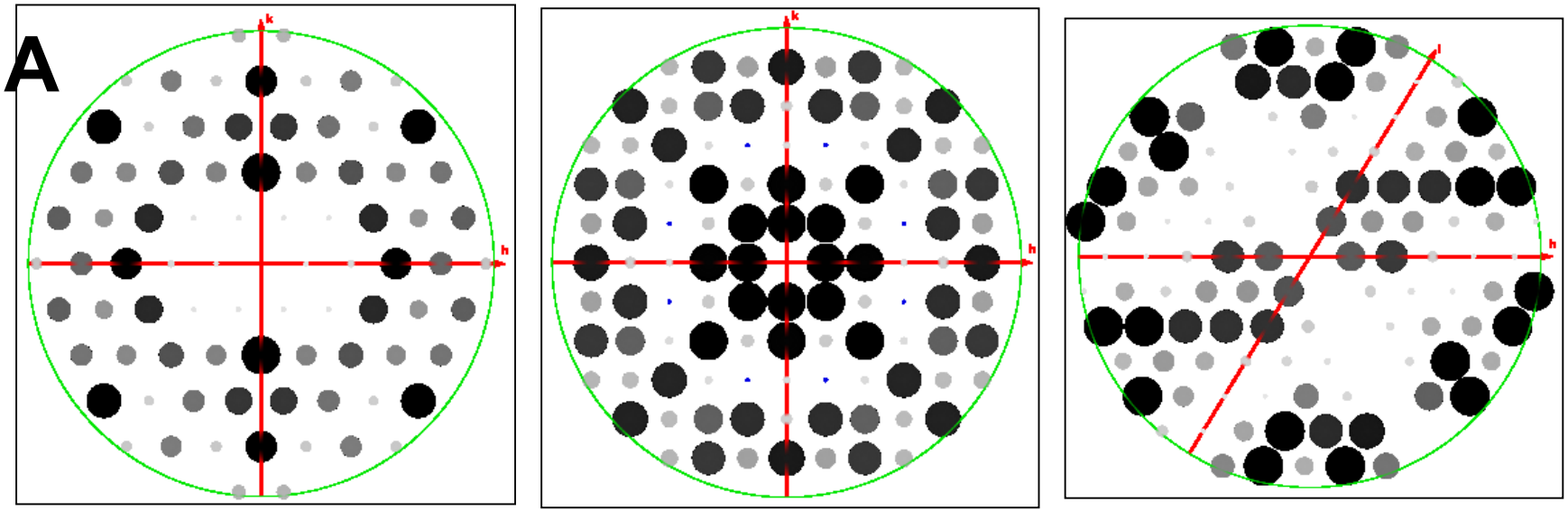
more degrees oscillation

+ less risk of spot overlap
- requires more exposures, time consuming
+ more accurate intensity measurements
0.5-1.0 degree for typical proteins

more risk of spot overlap -
requires fewer exposures, quicker collection +
less accurate measurements -
2.0 degrees for typical DNA oligos

Total Rotation Range

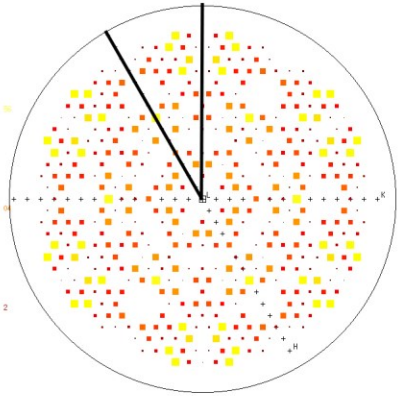
The 3 reciprocal lattices below reveal different degrees of rotational symmetry. Indicate the minimum amount of crystal rotation required to capture the unique part of each diffraction pattern: 45°, 90°, or 180°.



_____ _____ _____

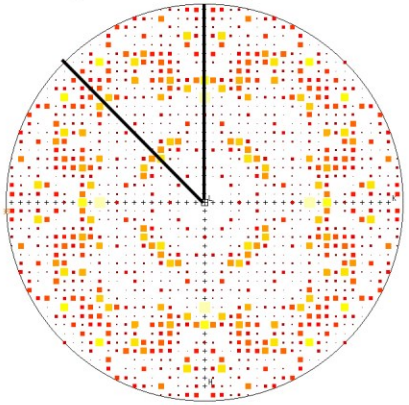
total number of **DEGREES** of rotation

30 degrees unique



P622 space group
(higher symmetry)

45 degrees unique



P422 space group
(lower symmetry)

fewer degrees of rotation

- risk lower completeness
- poor redundancy
+ quicker data collection
practical for high symmetry space groups

more degrees of rotation

completeness assured +
high redundancy +
time consuming to collect data -
required for low symmetry space groups