



Figure 1a

The Stoe Reciprocal Lattice Explorer is a new instrument, which incorporates the principle of both the Buerger Precession and the de Jong-Bouman methods. On the Explorer the alignment of the crystal and all photographs which are necessary for a space group determination can be taken in most cases with a single setting of the crystal. Only triclinic crystals have to be realigned on the instrument. The photographs show undistorted pictures of the reciprocal lattice planes which are taken with the same magnification.



Figure 1b

The Explorer has been designed

- for conveniently examining crystals prior to intensity measurements on automatic diffractometers
- for determining lattice constants of single crystals
- for rapid alignment of single crystals with Oscillation- or Buerger Precession  $\mu = 10^\circ$  (or  $\mu = 3^\circ - 5^\circ$ ) aligning photographs
- for teaching purposes

\* BD-Patent No 2 041 031, UK-Patent No 1 343 529, US-Patent No 119 102

**STOE**  
**Reciprocal  
 Lattice  
 Explorer\***



To comply with various requirements of crystallographers, Stoe produces two different versions of Reciprocal Lattice Explorers.

Figures 1a and 1b illustrate the Reciprocal Lattice Explorer 3.13.1 with a  $M = 60$  mm film to crystal distance for zero layer photographs as used in the de Jong-Bouman mode of operation (1a) and in the Buerger Precession mode of operation (1b).

Figures 2a and 2b illustrate the Reciprocal Lattice Explorer 3.14.1 with variable film to crystal distances of  $M = 75$  mm,  $M = 100$  mm and  $M = 125$  mm as used in the de Jong-Bouman mode of operation (2a) and in the Buerger Precession mode of operation (2b).



Figure 2a

## An application of the Reciprocal Lattice Explorer for space group determination

### 1) Alignment of the crystal

If the crystal has prismatic faces, it can be aligned with an accuracy of  $0.1^\circ$  by the telescope. If there are no faces, only the microscope is used for centering the crystal and the adjustment is made by Oscillation photographs, whereby the film cassette is parallel to the crystal rotation axis.

### 2) De Jong Bouman photographs ( $hk0$ , $hk1$ . . .)

For zero layer de Jong-Bouman photographs which are taken at  $\mu = 45^\circ$  the film cassette is perpendicular to the aligned crystal. The settings for higher layer photographs

are calculated with the lattice constant along the rotation axis, which is determined either from Oscillation photographs or from de Jong-Bouman Cone-Axis photographs. One circular diaphragm of 60 mm diameter is used in a fixed position for both zero layer and higher layer de Jong-Bouman photographs.

### 3) Buerger Precession photographs ( $0kl$ , $1kl$ . . . and $h0l$ , $h1l$ . . .)

For Buerger Precession photographs the film cassette has to be replaced into a position parallel to the crystal rotation axis.



Figure 2b

The photographs are taken in the same way as known from Precession Goniometers except that the angular positions of the crystal which are required for Precession photographs are already known from the preceding de Jong-Bouman photographs. In the triclinic case, adjustments of the arcs prior to Buerger Precession photographs are necessary which are controlled by  $\mu = 10^\circ$  (or  $\mu = 3^\circ - 5^\circ$ ) Buerger Precession aligning photographs.

The evaluation (indexing, lattice constant determination etc.) of Explorer photographs is very convenient, since all of them are undistorted pictures of reciprocal lattice planes taken with the same magnification.



## Constructional features of the Stoe Reciprocal Lattice Explorers

- High mechanical accuracy and stability.
- The angular position of the crystal can be read to  $0.1^\circ$  on a graduated drum with vernier.
- The distance between the film cassette and the crystal is set to an accuracy of 0.05 mm on a graduated film displacement mechanism. The film displacement mechanism can be easily changed from the de Jong-Bouman position to the Buerger Precession position which is also used for Oscillation photographs.
- The tilting angle  $\mu$  for de Jong-Bouman photographs and the Precession angle  $\mu$  are set on a segment to an accuracy of  $0.1^\circ$ .
- The layer line screen supports as used for de Jong-Bouman and for Buerger Precession photographs have two slots. Film packages for Cone-Axis photographs are inserted into the slots pointing towards the crystal, whereas the slots pointing towards the film cassette are used for the layer line screens. Thus Cone-Axis photographs can be taken simultaneously with zero layer de Jong-Bouman or Buerger Precession photographs.
- The position of the de Jong-Bouman diaphragm remains always in the same position whereas for Buerger Precession photographs the distance of the layer line screen from the crystal is conveniently set on a small scaled drum.
- A circular film cassette with an effective diameter of 120 mm which guarantees exactly planar films is used on the Explorer.
- A combined cutting and punching device is part of the accessories. The position of the film within the film cassette is determined by 4 holes in asymmetrical positions which are punched into the film.
- The plane which is determined by the crystal rotation axis and the X-Ray beam cuts de Jong-Bouman photographs in their equators as determined by 3 of the 4 punched holes if the reference mark on the film displacement mechanism coincides with the fixed reference mark on the support.
- The equators of Buerger Precession photographs are always parallel to the crystal rotation axis.
- The Explorer has 3 synchronous motors of which two are used for Oscillation or de Jong-Bouman photographs and the third is used for Buerger Precession photographs.
- A clutch on the crystal rotation axis has 3 positions: „Zero“ provides free rotation of the crystal, „de Jong“ engages the gear to the axle and „Buerger“ provides a fixed axle.
- The Explorer has two oscillation mechanisms of which one is used for Oscillation photographs and the other for Buerger Precession photographs.
- An electro-mechanical counter with zeroset records the number of oscillations and the number of revolutions if the Explorer is used in the Buerger Precession mode of operation. In the de Jong-Bouman mode of operation one revolution is indicated by two digits on the counter.

- A low background scattering is achieved by the use of concentric collimators of high precision which can be changed without readjustment of the instrument.
- A short collimator of 0.3 mm diameter is provided which is used if the arcs of the goniometer head are in extreme positions during exposures.
- A microscope-telescope-autocollimator system provides convenient working facilities. The microscope (50X) which is used for centering the crystals can be easily converted into a telescope with which the image of a Maltese cross with respect to a crosswire can be seen. The telescope provides an adjusting accuracy of  $0.1^\circ$  if the crystals have well developed prismatic faces.
- A precise and secure location of the Explorer during exposures is provided by lockable feet and bedding pads.

The variable Reciprocal Lattice Explorer 3.14.1 has a longer base plate which enables the operating parts with segment, displacement mechanism and support arm for the parallelogram to be moved against the stationary parts with the crystal rotation axis and the layer line screen support in a precise dovetail groove between  $M = 75$  mm over  $M = 100$  mm to  $M = 125$  mm. Parts of the instrument (e. g. layer line screen support, beam stop etc.) have been developed in cooperation with protein crystallographers. The result of this cooperation is an instrument which simplifies the operations as much as possible.

### Accessories included with all versions:

- 1 ACA standardised Goniometer head
- 1 microscope-telescope-autocollimator system
- 1 circular film cassette
- 1 combined cutting and punching device for circular films
- 3 bedding pads
- 1 layer line screen support for Buerger Precession photographs
- 1 wooden box containing
  - 1 layer line screen support for de Jong-Bouman photographs
  - 1 adjusting collimator
  - 3 collimators of 0.3, 0.5 and 0.8 mm diameters
  - 1 short collimator of 0.3 mm diameter
  - 1 beam stop with its adjusting device
  - 1 set of 4 layer line screens of 30, 40, 50 and 60 mm diameters of 3 mm slit width
  - 1 layer line screen of 60 mm diameter of 5 mm slit width
  - 2 paper insets for Cone-Axis photographs

### Additional accessories for the 3.14.1 model

- 1 adjusting screen with a central hole
- 1 special adjustable beam stop for protein photographs
- 1 set of additional layer line screens of 35, 45 and 55 mm diameters of 3 mm slit width
- 2 additional parallelograms
- Layer line screens of the mentioned diameters with 2 mm slit width can be ordered in addition.

Dimensions of the model 3.13.1:

Length 40 cm, width 55 cm, height 40 cm, weight 26 kg

Dimensions of the model 3.14.1:

Length 47 cm, width 55 cm, height 40 cm, weight 33 kg



## Attachments to the Stoe Reciprocal Lattice Explorers

### The Integrating Mechanism 0.43.1

enables precise intensity measurements in which irregularly shaped reflections on de Jong-Bouman and Buerger Precession photographs are spread along rectangular areas. The integrating mechanism has the shape of the circular film cassette and is fitted to the film displacement mechanism with the same bayonet clamp as the normal film cassette. Before being fitted, an axle must be inserted into the hollow displacement mechanism. The integration range can be continuously selected between zero and  $1,5 \times 1,5 \text{ mm}^2$ . The size is read on two scales. A complete integration range is finished after  $12 \times 12 = 144$  steps which are counted and displayed on the electro-mechanical counter with zeroset.

Figure 3 shows the Reciprocal Lattice Explorer in the de Jong-Bouman mode of operation on which the integrating mechanism is mounted.



Figure 3

### The XR-7-Polaroid-Land Diffraction Cassette 0.40.0

can be only used for Oscillation and Buerger Precession photographs and is fixed with the **special Adaptor 0.41.1** parallel to the crystal rotation axis. The Polaroid Cassette is suitable for taking quick adjusting photographs.

### The Circular Film Cassette with Intensifier Screen 0.40.5

for blue sensitive X-ray films shortens the exposure time. It is suitable for adjusting photographs.

## Further Stoe Products:

Computer Controlled Powder- and Single Crystal-Diffractometers

Position Sensitive Detectors

Curved and Flat X-Ray Monochromators

Guinier Cameras

Eulerian Cradles

Horizontal Diffractometers

Weissenberg Goniometers

Buerger Precession Goniometers

Optical Two-Circle Goniometers

Film Measuring Devices

Goniometer Heads

This description is submitted by: