XtaLAB mini

Desktop X-ray Crystallography System

1. Introduction

XtaLAB mini is a benchtop small molecule X-ray crystallography system. This chemical crystallography system is designed to produce publication quality structures automatically even though it is more compact and has lower power consumption (600 W) than its predecessor, the SCX-mini. Automated processing enables less-experienced users to determine crystal structures easily. X-ray crystallographic analysis has traditionally been regarded as one of the more difficult analysis methods, but with the XtaLAB mini, X-ray crystallographic analysis becomes as accessible as NMR and IR

2. Features

2.1. World's smallest diffractometer

A true benchtop system—dimensions are just 560×395×656 mm with a weight of approximately 100 kg. Easy to install almost anywhere.

2.2. Power saving

The generator operates at 600 W (approx. 1/4 of the power used by a conventional sealed tube system) leading to greatly reduced running costs. The XtaLAB mini uses a single phase power supply—no need for a 3-phase power supply.

No loss of intensity—use of the SHINE optic produces intensity comparable to a traditional (3 kW) system.

Fig. 1. Perspective view of XtaLAB mini.

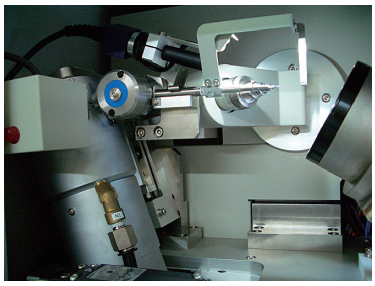


Fig. 2. Inside of XtaLAB mini.

2.3. Automatic measurement and analysis

System can be easily operated by everyone—auto mode allows all steps from data collection to the final structure report to be completed by doing nothing more than entering a chemical formula. Achievable data resolution and completeness meet IUCr publication

standards, and the system is capable of performing numerical absorption corrections.

2.4. Safety Design

Shutter ON–OFF interlock is linked to cabinet door—cabinet door can't be opened accidentally during X-ray on—no possibility of accidental X-ray exposure.

3. Software

XtaLAB mini comes with a comprehensive software package which automatically performs all necessary operations, from data collection to structure solution. This allows users without extensive experience in crystallography to determine crystal structures easily. In addition, the professional crystallographer can perform advanced manual operations using the CrystalClear software installed in high-end instruments.

Rigaku's proprietary structure solution package, CrystalStructure, is provided with the instrument. The package includes the following features:

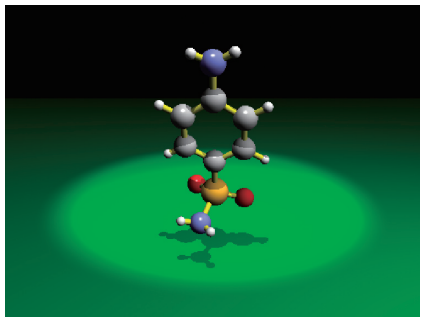
(1) Several determination programs for the initial phase: SIR, SHELX, SAPI, MULTAN, etc.
(2) Reliable structure refinement programs: CRYSTALS and SHELXL.
(3) One-click report and CIF generation.

The new version of CrystalStructure also includes the XPlain program, which automatically determines a structure's space group.

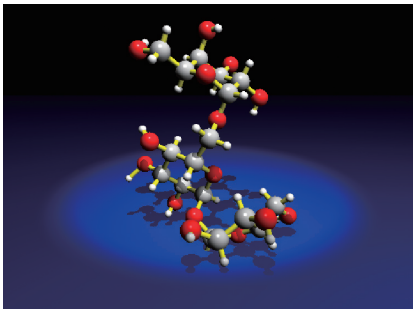
4. Specifications

Dimensions, Weight	560(W)×395(D)×656(H) mm, 100 kg
Rated output	600 W (Mo)
Optics	SHINE
Goniometer	Fixed χ:54°, 2θ:30°
	ω:2θ±90°(−60°～120°)
Video microscope	70x magnification - Displayed on PC
Sample to detector distance	Fixed at 50 mm
Detector area	ϕ 75 mm
Pixel size	73.2 μm/146.4 μm
Resolution	1024×1024 / 512×512
Read time	2.24/0.56 sec(1024/512)
PC OS	Windows XP

5. Applications



Sample	4- Aminobenzene sulfonamide
Formula	$C_6H_8N_2O_2S_1$
Formula weight	172.20
Sample size	0.40 X 0.32 X 0.28
Space group	$P2_1/c$
Lattice constants	a = 8.993 (6) Å
	b = 9.013 (5) Å
	c = 10.053 (6) Å
	β = 111.529 (8)°
	V = 757.9 (8) Å
	Z = 4
Measurement time	2h7min
R_{merge}	2.45%
R_1	3.21%



Sample	Raffinose
Formula	$C_{18}H_{32}O_{16}\cdot 5H_2O$
Formula weight	594.52
Sample size	0.25 X 0.13 X 0.12
Space group	$P2_12_12_1$
Lattice constants	a = 8.9700 (6) Å
	b = 12.3300 (9) Å
	c = 23.8100 (17) Å
	V = 2633.4 (3) Å
	Z = 4
Measurement time	5h30min
R_{merge}	6.74%
R_1	4.29%