Crystallographic analysis of microcrystals. III

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One of the current aims that we have for our experiments in hutch A of BL24XU is to evaluate the effectiveness of the combination of an unique undulator beam, simple optics and a cost-effective detector for microcrystal structure analyses. For the purpose of initial testing and training, we analyzed cytidine crystals.

Cytidine crystals were grown from ethanol and mounted on glass pins. An automatic pipette puller designed to make microelectrodes was utilized to prepare appropriate glass pins which were stiff enough and very thin at the tip. The diffraction data were collected at room temperature by an oscillation method. The data were reduced by PROCESS and structure refinement was done by SHELXL-93. Other computations were performed by teXsan.

The table summarizes the result. In conclusion, the current system installed in the experimental hutch A is useful for structure analyses of at least moderate size microcrystals of organic compounds.

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Table. Summary of experimental conditions and structure refinement.

Crystal	cytidine
Formula	$C_9H_{13}O_5N_3$
Crystal size (μm)	60 x 20 x 15
Delta φ (degree)	6.0
No. of total frames	20
Expo. time/fr. (min)	5
Space group	$P2_12_12_1$
a, b, c (Å)	14.0, 14.8, 5.1
Z	4
No. of reflections	
measured	4410
unique	1931
Rmerg	0.031
Resolution (Å)	0.81
Completeness (%)	93.1
Ref./param. ratio	12.3
R1, wR2	0.034, 0.090