

The lighter carbon and oxygen atoms have a very small contribution to the higher-order reflections, and the Fourier synthesis does not give accurate coordinates for these atoms. Further three-dimensional work is therefore planned. The other two projections are badly resolved and are not suitable for further structure analysis.

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### X-ray studies of molecular overcrowding. I. Some crystallographic data. By G. FERGUSON and G. A. SIM, *Chemistry Department, The University, Glasgow, W. 2, Scotland*

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With a view to obtaining detailed information about the effect on the molecular geometry of the close approach of neighbouring groups structural analysis of a number of substituted benzoic acids is at present in progress. As a preliminary to this work lattice parameters and space groups were determined and are presented in Table 1. In the case of *o*-chlorobenzoic acid and *o*-bromobenzoic

acid the diffraction conditions allow the space group to be either  $Cc-C_2^2$  or  $C2/c-C_{2h}^2$ . The successful refinement of the structure based on the centrosymmetrical choice indicates  $C2/c$  as the true space group.

Full details of the structure determinations will be published in due course.

Table 1. *Crystallographic data for some substituted benzoic acids*

Molecular formulae	<i>o</i> -chlorobenzoic acid $C_7H_5O_2Cl$	<i>o</i> -bromobenzoic acid $C_7H_5O_2Br$	2-chloro-5-nitro-benzoic acid $C_7H_4O_4NCl$	4-chloro-3-nitro-benzoic acid $C_7H_4O_4NCl$
<i>a</i> (Å)	14.73 ± 0.03	14.82 ± 0.04	5.86 ± 0.02	7.41 ± 0.02
<i>b</i> (Å)	3.90 ± 0.02	4.10 ± 0.02	5.13 ± 0.02	5.70 ± 0.02
<i>c</i> (Å)	25.50 ± 0.05	25.90 ± 0.05	26.65 ± 0.05	19.12 ± 0.04
$\beta$	112° 40'	118° 15'	97° 54'	100° 30'
<i>U</i> (Å <sup>3</sup> )	1351	1386	794	794
<i>z</i>	8	8	4	4
Mol. wt.	156.6	201.0	201.6	201.6
<i>D<sub>m</sub></i> (g.cm. <sup>-3</sup> )	1.544	1.929	1.678	1.687
<i>D<sub>x</sub></i> (g.cm. <sup>-3</sup> )	1.539	1.926	1.687	1.686
Space group	$C2/c-C_{2h}^6$	$C2/c-C_{2h}^6$	$P2_1/c-C_{2h}^2$	$P2_1/c-C_{2h}^2$

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### Unit cell and space group of L-proline monohydrate. By V. SASISEKHARAN, *Department of Physics, University of Madras, Madras-25, India.*

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Crystals of L-proline are highly hygroscopic. Therefore there has been considerable difficulty in growing single crystals suitable for X-ray diffraction studies. When grown from a saturated solution in a closed container, the crystals occur as a white powder or take up a feather-like formation, but no large enough single crystals appear at room temperature. The powder pattern obtained from this material was found to be very much different from that of the original compound thereby showing that the compound was a hydrated form of proline. The unit-cell dimensions and space group of the original dry powder have already been reported (Wright & Cole, 1949). Successful single crystals of the hydrated compound were grown by the author from a solution of the dry

material in ethyl alcohol by controlling the percentage of alcohol and the temperature at which the compound was crystallised. Single crystals of the monohydrate were obtained by dissolving the substance in 70% ethanol and keeping the solution at a constant temperature of 45 °C.

The crystals obtained were needle-shaped, transparent, birefringent and approximately rectangular in cross section. The needles were elongated along [001] and bounded by faces of the form {110}. As the crystals were unstable when exposed to the atmosphere, considerable care was taken to protect the crystals by enclosing them in Lindemann-glass tubes at 45 °C. Even then the crystals were stable for only a few days.