SOLVING CRYSTAL STRUCTURES FROM ELECTRON CRYSTALLOGRAPHY DATA VIA MAXIMUM ENTROPY AND LIKELIHOOD

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The maximum entropy (ME) method is ideal in these circumstances because:
(1) It will work, with projection data.
(2) It is stable regardless of data resolution.
(3) It uses non-uniform atomic distributions which are continually updated in the light of new phase information.
(4) It is not sensitive to data errors: this is important here where dynamical effects can produce systematic errors in intensity measurements.

We have applied the technique to both organics and inorganics including:
(b) Polyethylene, (Dorset, D.L. Macromolecules (1991) 24, 1175-1178)
(e) Copper porphyrins, (Dorset, D.L., Ultramicroscopy, (1991) 38, 41-45)
(f) Polybutene-1.

In cases the method has proved to work routinely.

MS-02.04.05 USE OF COHERENT ELECTRON DIFFRACTION AND COPIAL SCANNING IN OBTAINING DATA FOR DIRECT PHASING OF REFLECTIONS IN ELECTRON DIFFRACTION.

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The influence of dynamical scattering on electron diffraction data may be reduced by concentrating on higher order Laue zone (HOLZ) diffraction in convergent beam electron diffraction (CBED) data. Data obtained in this way has been used both to reduce atomic parameters with high accuracy and to solve structures by use of conditional Patterson transforms. As yet, only simple version of direct methods for phasing have been applied to limited data sets of intense reflections related by closed vector loops in centrosymmetric crystals (phase triplets with zero phase). In an attempt to reduce non-systematic