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A computer program to investigate reticular pseudomerohedry.

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The theory of twinning (Friedel, 1926) states that twinning on (*hkl*) by pseudomerohedry or reticular pseudomerohedry is likely to occur if the twin obliquity is less than 6° and the twin index does not exceed 5.

The twin obliquity is defined as the small angle between the normal to the net plane (*hkl*) and that row line [*uvw*] that is nearly normal ('quasi-normal') to (*hkl*).

The rotation that carries the lattice from its original orientation to the twinned orientation carries a certain fraction of the lattice points onto or near other lattice points. The reciprocal of the fraction of lattice points thus restored by twinning is the twin index. If it is unity one speaks of pseudomerohedry, otherwise of reticular pseudomerohedry. The twin index can be calculated as a simple function of the indices of the net plane and the row line (Donnay & Donnay, 1959).

Once the twin law of a given crystal has been ascertained, it is relatively easy to find the quasi-normal and compute the twin obliquity and the twin index, thus 'explaining' the twinning in terms of the theory. On the other hand, if one wishes to predict likely twin planes or twin axes from the theory, or indeed, to examine how well such predictions are borne out, then one needs to have a complete list of all those net-row combinations that are quasi-normal to one another and have low values of the twin index.

A computer program has been written to furnish such a complete list, since it is not easily obtained by graphical means or hand computation. The input data are the lattice parameters, the crystal system, the type of centering if any, and the maximum obliquity to be considered. The latter will usually be 6° or less, but any value may be used at the option of the user. The maximum twin index is fixed at 6, since a value greater than 5 need rarely be considered. The range of Miller indices is wide enough to insure completeness of the list, but an option exists to consider a smaller range at a great saving in execution time.

The printed output consists of six lists, one for each value of the twin index from 1 to 6. Each list gives pairs of net planes and row lines that are quasi-normal to one-another, the numerical value of the obliquity for each pair, and the direction angles for both plane and row.

The program is written in 7094 Fortran IV. All operating instructions are contained on comment cards at the head of the program listing. Interested parties in the U.S. and Canada may obtain a source deck by writing to the author. Requestors residing elsewhere will receive a listing of the program.

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Erratum: nuclear magnetic resonance in $BaCl_2.2H_2O$.

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In Table 1 (El Saffar, 1966) the neutron diffraction *r* values given in columns 2 and 3 should be interchanged. These *r* values are shown for purposes of comparison with the nuclear magnetic resonance results and have no bearing on the conclusions drawn.

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