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SORTHKL: Sort of Intensity Data as an Input Order of *h*, *k*, and *l*

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SORTHKL: 入力하는 *h*, *k*, *l*의 順序로 Intensity Data의 分類

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1. The Crystallographic Problem

Several thousands, sometimes, several tens of thousands of intensity data are needed for the elucidations of single crystal structures even for small molecules.

If so many intensity data are randomly arranged, it is almost impossible to confirm, by a visual measurement, the range of Miller indices detected, the duplications of reflections and more importantly the reflection conditions necessary for the space group determination.

The program SORTHKL sorts out any randomly arranged intensity data according to an arbitrary sequence of *h*, *k*, *l* to be input, where the first index varies first, and the second index second and the third index last.

2. How to Run the Program

(1) Click the sorthkl.exe two times with a mouse.

(2) The program will ask you, on your monitor, the name of an input intensity data file preferably with a format 3*I*4, 2*F*8.2.

Just click after writing the input file name

(3) The program will ask you the name of an output file.

Just click after writing the output file name

(4) The program will ask you the order of *h*, *k*, *l*.

Just click after writing *h*, *k*, *l* in order you want to vary them (e.g. *l*, *k*, *h*).

Then the program will automatically create an output file you named, in which the data are written in the format 3*I*4, 2*F*8.2 commonly used for crystal structure analyses.

3. Software and Hardware Environment

The program SORTHKL is written in Fortran90 and will run on a PC.

The maximum executable number of the intensity data is currently 200,000, but it is possible to expand.

4. Documentation and Availability

Copy of the program is available via e-mail from ihsuh@korea.ac.kr.

5. Keywords

Single crystal, Intensity data, Crystal structure analyses.