33. *On the Crystallographic Space Groupoid*

By Tei-ichi ITO, M. J. A., and Ryoichi SADANAGA
Mineralogical Institute, Faculty of Science, University of Tokyo

(Comm. March 12, 1976)

Some crystal structures are known to have local symmetry elements besides ordinary space-group (global) symmetry elements (Ito, 1950). A complete set of these local symmetry operations and global ones, both operating on one and the same crystal structure, constitute a groupoid defined by Brandt (1926) (Dornberger-Schiff, 1957). However, no clear-cut definition of the crystallographic space groupoid has yet been presented, and accordingly the study to find out the proper position for twinned space groups (Ito, 1935, 1950) in the classes of crystallographic space groupoids has been left intact. In this report we shall deal with these problems.

There exist such partitions of the Euclidean three-space that give rise to polyhedra which are congruent with each other but not related with each other by space-group operations (Hilbert, 1935; Reinhardt, 1928). A point system derived from such a partition is here designated as *hyporegular*. Then, a crystallographic space groupoid must satisfy the condition that the point system derived from it be such a hyporegular point system that can be partitioned into classes of regular point subsystems. Since the structure under consideration is crystallographic, it must conform to a space group to begin with. Therefore, every point in the hyporegular point system must form, with points equivalent to it according to the space-group symmetry, a regular point subsystem. On the other hand, because every crystal structure is built up by dense packing of fundamental regions, it will be a natural extension of this concept that the point system derived from a crystallographic space groupoid is at least hyporegular, its polyhedra forming the fundamental regions for the space groupoid. An example is illustrated in Fig. 1 for a unit cell *ABCD* of such a hyporegular point system as described above. However, because no actual crystal structure according to this symmetry principle has ever been discovered, we denote a space groupoid with this property as *quasi-crystallographic*.

In order to approach significant descriptions of actual crystal structures, we specify the quasi-crystallographic space groupoid by introducing a condition that a congruent embedding exists from a simply connected subspace of a certain regular point system onto a