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## *A method to obtain all geometric ambiguities in powder indexing*

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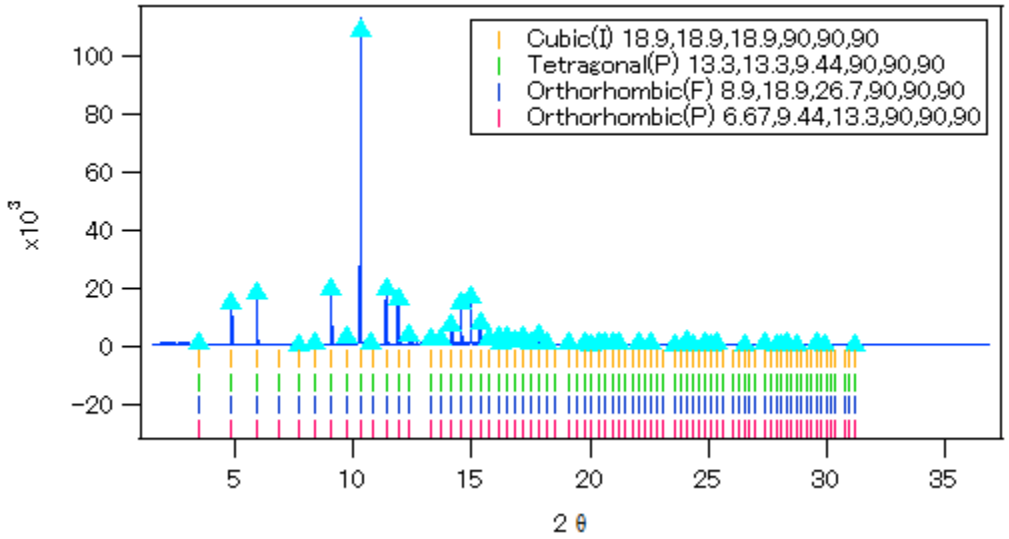
It is known that different unit cells can have the same computed lines in some cases (Figure). The phenomenon was first called geometrical ambiguity and studied in [1]. In all the high-symmetric cases provided in [1], such unit cells correspond to derivative lattices of each other. Although this is not true in general for 3-dimensional lattices, this has been assumed in methods to search for geometrical ambiguities (e.g., [2]). Thus, a method to obtain all the geometrical ambiguities in very short time for a given unit cell parameters is provided. Because such a method has not been used for powder indexing, it will have impact in the following sense: firstly, it is useful for checking powder indexing solutions promptly. Some powder auto-indexing methods cannot obtain all the geometrical ambiguities. Even for the software including Conograph which can gain all the ambiguities, it is not straightforward to search for them from many indexing solutions using the figures of merit which are sometimes not reliable [3]. Secondly, the new method indicates that powder indexing has only finitely many solutions at least if peak search succeeds in obtaining all (but a few) diffraction peaks with q-values smaller than some calculated value. (Note that infinitely many solutions may exist for lattices of dimension more than 4.) The result seems to provide a foundation of automatic powder crystal structure analysis, because it is possible to obtain all the ambiguities by computation. The introduced method was implemented in the newest version of Conograph, which will be distributed on the web (http://research.kek.jp/people/rtomi/ConographGUI/web_page.html) by IUCr2014. ACKNOWLEDGEMENT: this research was partly supported by a JSPS KAKENHI grant (No.22740077) and by Ibaraki Prefecture (J-PARC-23D06).

***[1]*** *A. D. Mighell & A. Santoro, J. Appl. Cryst., 1975, 8, 372-374,* ***[2]*** *H. Kroll et. al., J. Appl. Cryst., 2011, 44, 812-819,* ***[3]*** *R. Oishi-Tomiyasu, J. Appl. Cryst., 2013, 46, 1277-1282*

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