

## 蛋白质结晶学中纯直接法的新进展

侯永庚,陈建信,赵cheng,李立璞

中国科学院化学研究所.北京(100080);中国科学院分子动态与稳态结构国家重点实验室

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### 摘要

纯直接法是一种abinitio方法。它只用X射线实验得到的有原子分辨率的母体数据和单胞中原子种类及数目就能解出小蛋白质的结构位相。目前流行的双空间法SnB和SHELX-D, 根据整体极小化原理设计、运用倒易空间位相修正和正空间密度修饰交替迭代的策略已能解含1001

个非H肽原子的溶菌酶结构。我们采用系统论和优化法的思想与结构不变量的概率分布理论相结合, 研究成功了在倒易空间直接求解位相的系统优化法及程序SYSTEM-99。用它测定了0.110nm分辨率含1914个不重于S的非H肽原子的天花粉(TCS)结构的初始模型。

关键词 [蛋白质](#) [结晶](#) [从头计算法](#) [目标函数](#) [系统优化法](#)

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## New developments in 'pure' direct methods for protein crystallography

Hou Yonggeng, Chen Jianxin, ZHAO che, Li Lipu

Inst of Chem, CAS, Beijing(100080)

**Abstract** 'pure' direct method is an ab initio method. Recent advances in ab initio direct methods have enabled the solution of crystal structure of small protein from the type and number of atoms in cell as well as native X-ray data that must be available to atomic resolution, that is, without the use of fragments of known structure or the need to prepare heavy-atom derivatives. An approach that is gaining rapidly in popularity is dual space recycling methods SnB and SHELX-D. They have recently solved the previously known structure of triclinic lysozyme consisting of 1001 non-H protein atoms, none heavier than sulfur. The system optimization method has developed from the integration of systematization, optimization and the probability distribution of structure-invariant. Its program is called SYSTEM-99. On it there is one effective objective function, which is out of ordinary, according to size of the structure, intensity and extensity of relations between reflections, it divides reflections into many subsystems. Then by means of minimization in objective function, it determines all the phases among subsystem in reciprocal space. The SYSTEM-99 program was able to solve the structure of trichosanthes root (TCS) that contains with 1914 non-H protein atoms none heavier than sulfur.

**Key words** [PROTEIN](#) [CRYSTALLIZE](#) [AB INITIO CALCULATION](#)

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