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大别山绿辉石晶体结构的再研究—兼与谢奕克等同志商榷 [点此下载全文](#)

[郭卫东](#) [罗谷风](#)

南京大学地球科学系(郭卫东, 罗谷风)
, 南京大学地球科学系(郭昀)

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摘要:

谢奕克等曾测定了大别山一个绿辉石的晶体结构, 认为它具 $P2/c$ 空间群; 四面体链分别呈 SA 和 OB 配位的八面体; $A1$ 在所有这四种晶位另均有相当多的占有率, 为绿辉石的新型结构。本文对该资料再研究后确认结构中仅有一种 O 旋转的四面体链; $M2$ 和 $M2(1)$ 晶位为 8 次配位; $A1$ 全部进入 $M1(1)$ 晶位, $A1-Mg$ 呈完全有序绿辉石。本文给出了重新计

关键词: [绿辉石](#) [空间群](#) [晶体结构](#) [大别山](#)

RESTDY ON THE CRYSTAL STRUCTURE OF OMPHACITE FROM THE DABIE MOUNTAINS [Download Full](#)

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Abstract:

Xie Douke et al. (1989) determined the crystal structure of omphacite from the Dabie Mountains. This crystal has space group $P2/c$, and in its structure, there are two kinds of tetrahedral chain with rotation respectively; the four symmetrically unequivalent M-sites are all 6-coordinated octahedra with higher occupancies. A restudy on the data of this structure was carried out by the authors. The space group of the omphacite from the Dabie Mountains is $P2/n$ rather than $P2/c$; and in its structure of tetrahedral chain with 0-rotation, the 03-03-03 chain angle is 170.02° and $M2$ and $M2(1)$ sites are distinguished from 6-one of $M1$ and $M1(1)$ sites. In addition, the authors deem that, based on the $M1$ structure mentioned above is a typical one of ordered omphacite with space group $P2/n$, rather than for omphacite. The cause responsible for an incorrect space group is that the selection of the unit cell is not the standard. The authors, therefore, recalculated the unit cell parameters and atom coordinates based on the data given by Xie Douke et al., and furnish the correct ones here. Although some major errors have been found in given by Xie Douke et al., the structural data are valuable.

Keywords: [omphacite](#) [space group](#) [crystal structure](#) [Dabie Mountains](#)

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