ABSTRACT

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Polymorphism of $CsGaSe_2$

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The crystal structure of $CsGaSe_2$ was redetermined by single-crystal X-Ray diffraction. It confirmed the results reported by *Deiseroth* et al.[1] The title compound crystallizes in two polymorphic modifications.[1, 2] Both modifications crystallize monoclinically in the space group *C*2/*c* (No. 15) with a = 7.6472(3) Å, b = 12.5315(4) Å, c = 6.1664(2) Å, β = 113.736(4)°, V = 540.94(4) Å^3, and Z = 4 for $CsGaSe_2$-I,[2] and a = 11.030(1) Å, b = 11.033(1) Å, c = 16.803(1) Å, β = 99.43(1)°, V = 2017.1(3) Å^3, and Z = 16 for $CsGaSe_2$-II.[2]

The anionic substructure of $CsGaSe_2$-I consists of infinite one-dimensional chains <brol>1<brtr>∞</brol>$GaSe_2^-$] composed of edge sharing $GaSe_4$ tetrahedra (Figure 1). $CsGaSe_2$-II shows layers of vertex sharing supertetrahedral Ga_4Se_{10}-units composed of four corner sharing $GaSe_4$ tetrahedra (Figure 1).

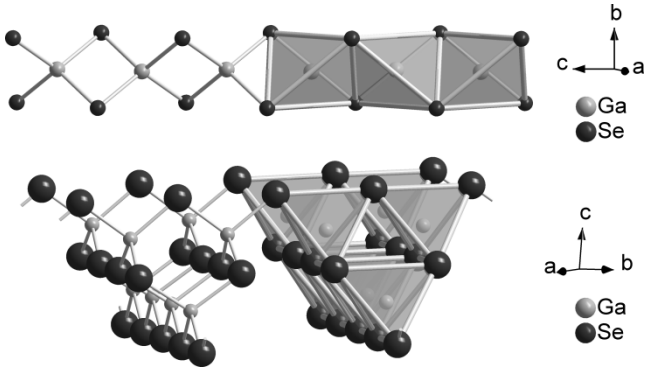

Figure 1. Section of the anionic substructres of both $CsGaSe_2$ polymorphs, showing the characteristic tetrahedra linkage in $CsGaSe_2$-I (top) and $CsGaSe_2$-II (bottom) .

[1] H. J. Deiseroth, *Z. Kristallogr.* **1984**, *166*, 283.
[2] A. Kyas, Dissertation, TH Aachen **1981**.