Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supplementary Information for the manuscript

Polymorphism of $CsGaS_2$ – Structural Characterization of a new two-dimensional Polymorph and Study of the Phase-Transition Kinetics

*Daniel Friedrich, Marc Schlosser, Richard Weihrich and Arno Pfitzner**

*Prof. Dr. Arno Pfitzner

Institut für Anorganische Chemie, Universität Regensburg, Universitätsstraße 31, 93040 Regensburg, Germany

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Table S1 Anisotropic displacement parameters U_{ij} (in Å^2) for $CsGaS_2$-*mC*64.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cs1	0.0206(2)	0.0222(2)	0.0166(2)	-0.0050(1)	0.0027(1)	-0.0002(1)
Cs2	0.0201(2)	0.0213(2)	0.0177(2)	0.0049(1)	0.0033(1)	-0.0003(1)
Ga1	0.0111(2)	0.0120(3)	0.0105(2)	0.0014(2)	0.0025(2)	-0.0004(2)
Ga2	0.0107(2)	0.0121(3)	0.0106(2)	-0.0011(2)	0.0017(2)	-0.0004(2)
S1	0.0138(5)	0.0148(7)	0.0100(5)	-0.0056(4)	0.0019(4)	0.0000(5)
S2	0.0126(5)	0.0125(7)	0.0104(5)	0.0062(4)	0.0022(4)	-0.0001(5)
S3	0.0098(5)	0.0130(8)	0.0146(6)	-0.0004(4)	0.0027(4)	-0.0023(4)
S4	0.0141(7)	0.0126(1)	0.0129(7)	0	0.0049(6)	0
S5	0.0129(7)	0.0126(1)	0.0134(7)	0	-0.0001(6)	0

Table S2 Selected interatomic distances /Å and angles /° for $CsGaS_2$-*mC*64.

Bond length / Å				Angle /°	
Ga1-S1^{vii}	2.300(1)	Cs1-S1	3.749(1)	S1^{vii}-Ga1-S2	108.24(4)
Ga1-S2	2.304(1)	Cs1-S1^{viii}	3.743(1)	S1^{vii}-Ga1-S3	110.25(5)
Ga1-S3	2.260(1)	Cs1-S1^{ii}	3.488(1)	S1^{vii}-Ga1-S4	110.22(4)
Ga1-S4	2.260(1)	Cs1-S2^{v}	3.535(1)	S2-Ga1-S3	107.28(4)
Ga2-S1	2.304(1)	Cs1-S3	3.552(1)	S2-Ga1-S4	107.30(5)
Ga2-S2^{xiii}	2.308(1)	Cs1-S3^{iv}	3.555(1)	S3-Ga1-S4	113.34(4)
Ga2-S3	2.261(1)	Cs1-S4	3.552(1)	S1-Ga2-S2^{xiii}	108.62(4)
Ga2-S5	2.260(1)	Cs1-S5^{viii}	3.556(1)	S1-Ga2-S3	110.16(5)
		Cs2-S1^{xii}	3.512(1)	S1-Ga2-S5	110.15(4)
Cs1-Cs1^{i}	5.256(1)	Cs2-S2	3.741(1)	S2^{xiii}-Ga2-S3	107.17(4)
Cs1-Cs1^{ii}	5.257(1)	Cs2-S2^{xi}	3.747(1)	S2^{xiii}-Ga2-S5	107.20(5)
Cs1-Cs2^{iii}	3.746(1)	Cs2-S2^{x}	3.566(1)	S3-Ga2-S5	113.35(4)
Cs1-Cs2^{iv}	3.730(1)	Cs2-S3	3.508(1)		
Cs1-Cs2^{v}	5.273(1)	Cs2-S3^{iii}	3.508(1)		
Cs1-Cs2^{vi}	5.275(1)	Cs2-S4^{xi}	3.506(1)		
Cs2-Cs2^{iii}	4.676(1)	Cs2-S5^{viii}	3.511(1)		
Cs2-Cs2^{ix}	5.297(1)				
Cs2-Cs2^{x}	5.295(1)				

[a] Symmetry codes used to generate equivalent atoms: (i) -x+1,-y,-z+1; (ii) -x+0.5,-y+0.5,-z+1; (iii) -x+1,y,-z+0.5; (iv) -x+0.5,y-0.5,-z+0.5; (v) x,-y,z+0.5; (vi) x-0.5,-y+0.5,z+0.5; (vii) -x,y,-z+0.5; (viii) x+0.5,y-0.5,z; (ix) -x+1,-y+1,-z; (x) -x+0.5,-y+0.5,-z; (xi) x+0.5,y+0.5,z; (xiii) -x+0.5,y+0.5,-z+0.5.

Table S3 Anisotropic displacement parameters U_{ij} (in Å^2) for $CsGaS_2$-*mC*16.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cs	0.0144(1)	0.0128(1)	0.0152(1)	0	0.0057(1)	0
Ga	0.0097(1)	0.0111(1)	0.0067(1)	0	0.0042(1)	0
S	0.0128(2)	0.0129(2)	0.0095(2)	0.0032(1)	0.0055(1)	0.0016(1)

Table S4 Selected interatomic distances /Å and angles /° for $CsGaS_2$-*mC*16.

Bond length / Å				Angle /°	
Ga-S	2.2869(5)	Cs-S	3.6200(5)	S-Ga-S^{vii}	112.44(2)
Ga-S^{xii}	2.2823(4)	Cs-S^{v}	3.6813(5)	S-Ga-S^{xii}	99.54(2)
		Cs-S^{vii}	3.6200(5)	S-Ga-S^{xiv}	114.30(2)
Ga-Ga^{xii}	2.9510(2)	Cs-S^{viii}	3.6813(5)	S^{vii}-Ga-S^{xii}	114.30(2)
		Cs-S^{ix}	3.7025(5)	S^{vii}-Ga-S^{xiv}	99.54(2)
Cs-Cs^{i}	4.5850(3)	Cs-S^{iv}	3.6812(5)	S^{xii}-Ga-S^{xiv}	117.44(2)
Cs-Cs^{iii}	4.5032(3)	Cs-S^{x}	3.6812(5)		
		Cs-S^{xi}	3.7025(5)		

[a] Symmetry codes used to generate equivalent atoms: (i) -x,-y,-z; (iii) -x-0.5,-y+0.5,-z; (iv) -x+0.5,-y+0.5,-z+1; (v) x-0.5,y-0.5,z; (vii) -x,y,-z+0.5; (viii) -x+0.5,y-0.5,-z+0.5; (ix) -x+0.5,-y+0.5,-z; (x) x-0.5,-y+0.5,z-0.5; (xi) x-0.5,-y+0.5,z+0.5; (xii) -x,-y+1,-z; (xiv) x,-y+1,z+0.5.

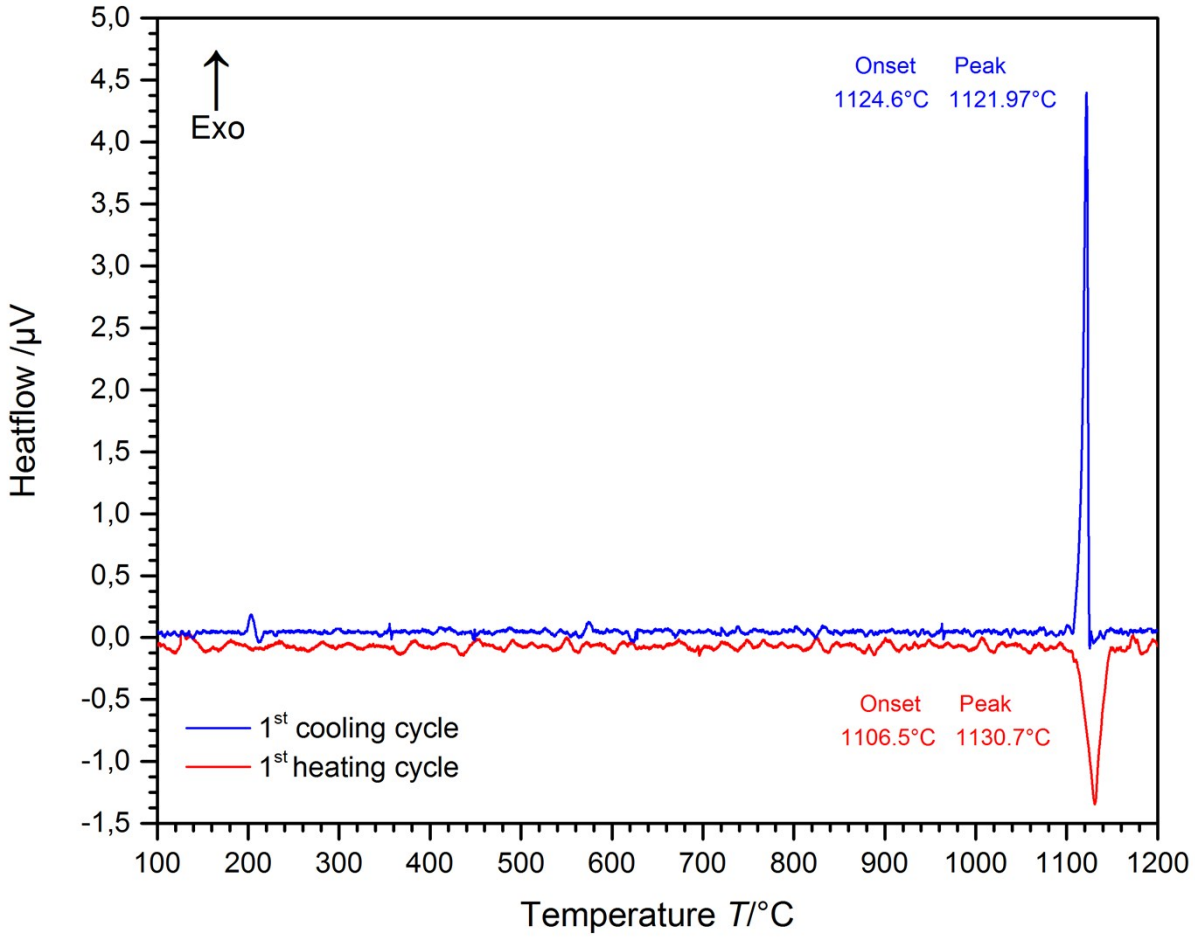

Figure S1 Differential thermal analysis (DTA) of $CsGaS_2$-*mC*16 (the baseline was manually subtracted). Heating rate is 10 K/min.

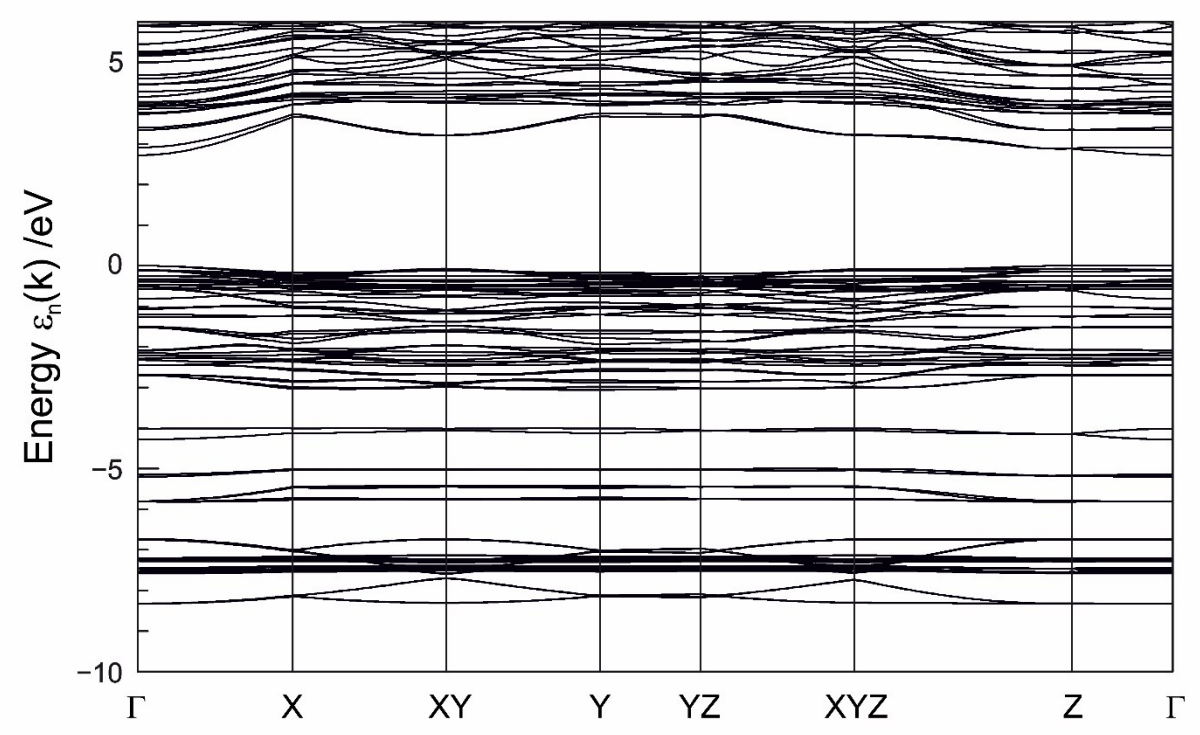

Figure S2 Electronic band structure of $CsGaS_2$-*mC*64.

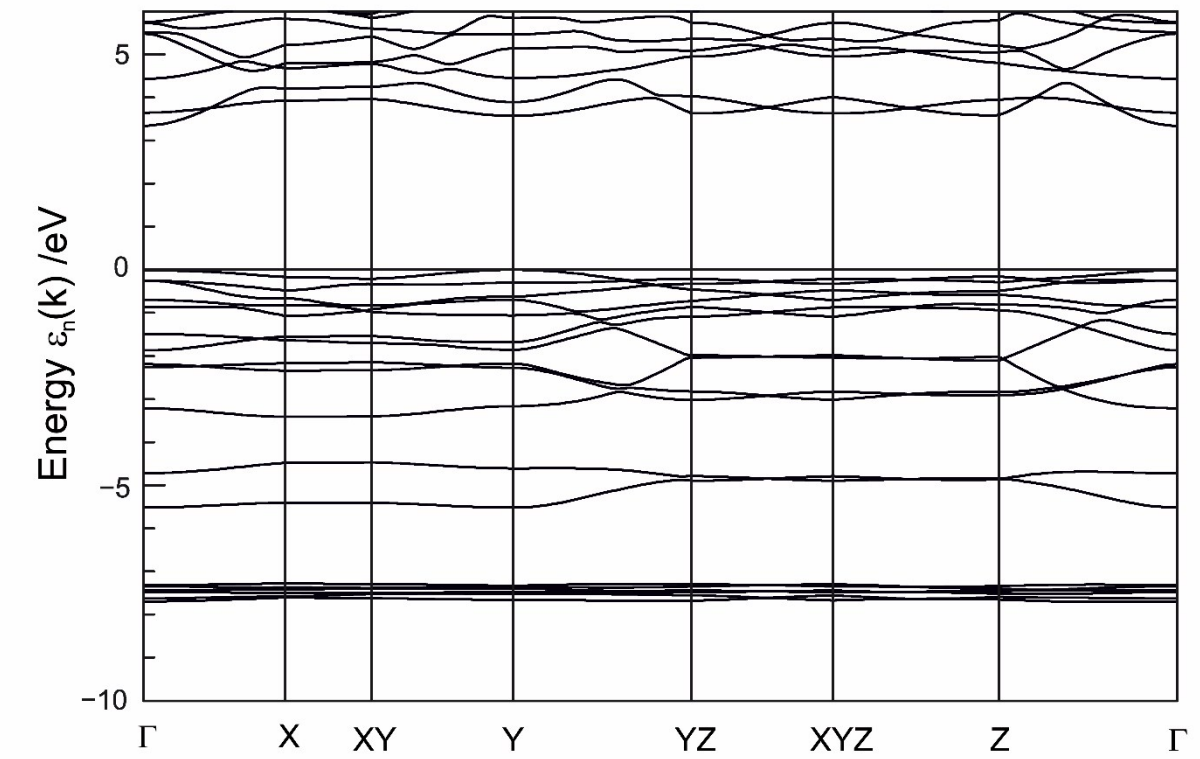

Figure S3 Electronic band structure of $CsGaS_2$-*mC*16.