# Semiconducting Behavior of Type-I Si Clathrate

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## Supplementary Material

Table S1. Experimental and refined details for the single-crystal measurements. S2
Table S2. Atomic positions and displacement parameters of $K_8Ga_{16}Si_{38}$. S4

S1. Experimental and refined details for the single-crystal measurements.

| | |
|---|---|
| Crystal data | |
| Chemical Formula (Structural analysis) | $K_8Ga_{8.3(1)}Si_{37.7}$ |
| $M_r$ | 1950.283 |
| Crystal color | Gray, Metallic luster |
| Crystal size (mm) | 0.20 x 0.15 x 0.04 |
| Temperature (K) | 293 |
| Space group | $Pm\bar{3}n$ (No. 223) |
| A (Å) | 10.4261(2) |
| V (Å$^3$) | 1133.35(4) |
| Z | 1 |
| $D_x$ (g/cm$^3$) | 2.858 |
| $\mu$(MoK$\alpha$) (cm$^{-1}$) | 6.580 |
| | |
| Data Collection | |
| Radiation | MoK$\alpha$ ($\lambda$ = 0.71073 Å) |
| Diffractometer | Bruker SMART APEX CCD |
| Data collection method | $\omega$ scans |
| Absorption correction | Empirical<br>SADABS in SAINT-Plus-NT |
| $T_{min}$, $T_{max}$ | 0.3612, 0.5276 |
| $2\theta_{max}$ (°) | 61.04 |
| No. of measured, independent and observed reflections | 8352, 338, 321 |
| $R_{int}$ | 3.15 |
| | |
| Refinement | |
| No. of parameters | 19 |
| Refinement on | $F^2$ |
| $R[F^2>2\sigma(F^2)]$, $wR(F^2)$, $S$ | 1.30, 3.27, 1.098 |
| Weighting scheme | $w = 1/[\sigma^2(F_O^2) + (0.0381P)^2]$, where $P = (F_O^2+2F_C^2)/3$ |
| $(\Delta/\sigma)_{max}$ | 0.001 |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (eÅ$^{-3}$) | 0.27, -0.30 |

Programs

Data collection: SMART-NT (Bruker, 1999) [S1.1]; cell refinement: SAINT-Plus-NT (Bruker, 1999) [S1.2]; data reduction: SAINT-Plus-NT (Bruker, 1999) [S1.2]; program used to refine structure: SHELXL-97 (Sheldrick, 1997) [S1.3].

References

[S1.1] Bruker (1999). SMART-NT. Version 5.625. Bruker AXS Inc., Madison, Wisconsin, USA.

[S1.2] Bruker (1999). SAINT-plus-NT. Version 6.45. Bruker AXS Inc., Madison, Wisconsin, USA.

[S1.3] G.M. Sheldrick, A short history of SHELX, Acta Cryst. **A64** (2008) 112-122.

S.2 Atomic positions and displacement parameters of $K_8Ga_{16}Si_{38}$.

| Atom | Multiplicity Wyckoff Letter | x | y | z | Occ. | $U_{eq}$ |
|---|---|---|---|---|---|---|
| K1 | 2a | 0 | 0 | 0 | 1 | 0.0127(2) |
| K2 | 6d | 1/4 | 1/2 | 0 | 1 | 0.0266(2) |
| E1 | 6c | 1/4 | 0 | 1/2 | 0.607(5) Ga<br>0.393 Si | 0.0097(1) |
| E2 | 16i | 0.18442(2) | x | x | 0.026(2) Ga<br>0.974 Si | 0.0088(2) |
| E3 | 24k | 0 | 0.30577(2) | 0.11804(3) | 0.179(2) Ga<br>0.821 Si | 0.0095(1) |

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| K1 | 0.0127(2) | $U_{11}$ | $U_{11}$ | 0 | 0 | 0 |
| K2 | 0.0179(3) | 0.0310(3) | $U_{22}$ | 0 | 0 | 0 |
| E1 | 0.0107(2) | 0.0092(2) | $U_{22}$ | 0 | 0 | 0 |
| E2 | 0.0088(2) | $U_{11}$ | $U_{11}$ | -0.00051(8) | $U_{12}$ | $U_{12}$ |
| E3 | 0.0092(2) | 0.0098(2) | 0.0096(2) | 0 | 0 | -0.00018(9) |