**STRUCTURE REPORT**

**Crystallographer:** F. Engelhardt

**ID code:** IDCODE Date: 09.11.2017

**Sample by:** Julia Bastian

**Compound:**

**Formula sum:** 'C18 H54 Cl Ge N3 Si6'

**Formula moieties:** 'C18 H54 Cl Ge N3 Si6'

PICTURE

**Figure 1**. Molecular structure of the title compound in the crystalline state. Thermal ellipsoids of the heavier atoms with 50% probability, H atoms omitted for clarity.

**Crystallographic Data and Details on Structure Refinement**

formula sum 'C18 H54 Cl Ge N3 Si6'

formula weight 589.22

crystal size (mm) 0.14 x x 0.25 mm

crystal system trigonal

space group SPGRP

unit cell parameters

a (Å) 17.798(7)

b (Å) 17.798(7)

c (Å) 16.815(9)

α (deg)

β (deg) 90

γ (deg) 120

unit cell volume V (Å3) 4613(4)

molecules per cell z 6

crystallographic density μ calcd (g cm-3) 1.273

absorption coefficient µ (mm-1) 1.329

diffractometer STOE IPDS 2T

radiation (λ [Å]) graphite-monochromated Mo-Kα (0.71073)

temperature (°C) -173.15

scan type ω scan (increment 1.5°, exposure 1 min)

completeness of dataset 0.998%

θ range of data collection (deg) 2.289 to THETAMAX

reflections collected 9039

independent reflections 2744

independent reflections with I>2σ(I) 27442S

structure solution method dual-space structure solution (SHELXT)

refinement method full-matrix least-squares on F2 (SHELXL 2016/4)

absorption correction method numerical

range of transmission factors TMAX and 0.6847

data / parameters / restraints DATA / PARAM / 1

goodness of fit (GooF) [all data] 1.148

final R values

R1 [all data, I ≥ 2σ (I)] R1ALL, 0.0238

wR2 [all data, I ≥ 2σ (I)]] WR2ALL, 0.0538

largest difference peak and hole 0.629 and DEEPHOLE eÅ-3

Refinement special details:

none