

### General

**Origin** Cs<sub>8</sub>Na<sub>10</sub>Tl<sub>6</sub>Ge<sub>136</sub>

### Bibliographic data

### Phase data

**Space-group** C 1 2/m 1 (12) - monoclinic

**Cell** a=21.9114 Å b=21.9114 Å c=26.8359 Å β=144.74°

V=7438.68 Å<sup>3</sup>

### Atomic parameters

Atom	Ox.	Wyck.	Site	S.O.F.	x/a	y/b	z/c	U [Å <sup>2</sup> ]
Cs1		8j	1		0.25000	0.25000	0.87500	0.0343
Na2		8j	1		0.37500	-0.12500	0.75000	0.0155
Tl3		8j	1		0.12500	0.12500	0.25000	0.0155
Ge4		8j	1		0.25000	-0.25000	0.37500	0.0082
Ge5		8j	1		0.25000	-0.25000	0.28262	0.0089
Ge6		8j	1		0.59238	0.09238	0.96738	0.0089
Ge7		8j	1		0.34238	0.34238	0.46738	0.0089
Ge8		8j	1		0.56524	0.25000	0.28262	0.0089
Ge9		8j	1		0.34238	0.15762	0.46738	0.0089
Ge10		8j	1		0.40762	0.40762	0.03262	0.0089
Ge11		8j	1		0.09399	0.09399	0.81768	0.0096
Ge12		8j	1		0.34399	-0.15601	0.31768	0.0096
Ge13		8j	1		0.59399	0.09399	0.81768	0.0096
Ge14		8j	1		0.34399	0.34399	0.31768	0.0096
Ge15		8j	1		0.65131	0.15131	0.93232	0.0096
Ge16		8j	1		0.40131	0.40131	0.43232	0.0096
Ge17		8j	1		0.54137	0.15601	0.31768	0.0096
Ge18		8j	1		0.79137	-0.09399	0.81768	0.0096
Ge19		8j	1		0.29137	-0.09399	0.81768	0.0096
Ge20		8j	1		0.21333	0.09869	0.43232	0.0096
Ge21		8j	1		0.71333	0.09869	0.43232	0.0096
Ge22		8j	1		0.40131	0.09869	0.43232	0.0096
Ge23		8j	1		0.46333	0.15131	0.93232	0.0096
Ge24		8j	1		0.54137	0.34399	0.31768	0.0096
Ge25		8j	1		0.56201	0.25000	0.12969	0.0096
Ge26		8j	1		0.44737	0.25000	0.12969	0.0096
Ge27		8j	1		0.49531	0.19268	0.62031	0.0096
Ge28		8j	1		0.49531	-0.30732	0.62031	0.0096

Ge29	8j	1	0.74531	0.05732	0.12031	0.0096
Ge30	8j	1	0.34869	0.34869	0.06768	0.0096
Ge31	8j	1	0.53667	-0.34869	0.06768	0.0096
Ge32	8j	1	0.75469	-0.05732	0.87969	0.0096
Cs33	4i	m	1/2	0	3/8	0.0343
Cs34	4i	m	0	0	3/8	0.0343
Na35	4i	m	1/4	0	0	0.0155
Ge36	4i	m	0	0	7/8	0.0082
Ge37	4i	m	1/2	0	7/8	0.0082
Ge38	4i	m	0	0	0.78262	0.0089
Ge39	4i	m	1/2	0	0.78262	0.0089
Ge40	4i	m	0.81524	0	0.78262	0.0089
Ge41	4i	m	0.31524	0	0.78262	0.0089
Ge42	4i	m	0.81201	0	0.62969	0.0096
Ge43	4i	m	0.31201	0	0.62969	0.0096
Ge44	4i	m	0.69737	0	0.62969	0.0096
Ge45	4i	m	0.19737	0	0.62969	0.0096
Na46	2a	2/m	0	0	0	0.0155
Tl47	4f	-1	1/4	-1/4	1/2	0.0155
Na48	2b	2/m	1/2	0	0	0.0155
Na49	4h	2	1/2	-1/4	1/2	0.0155

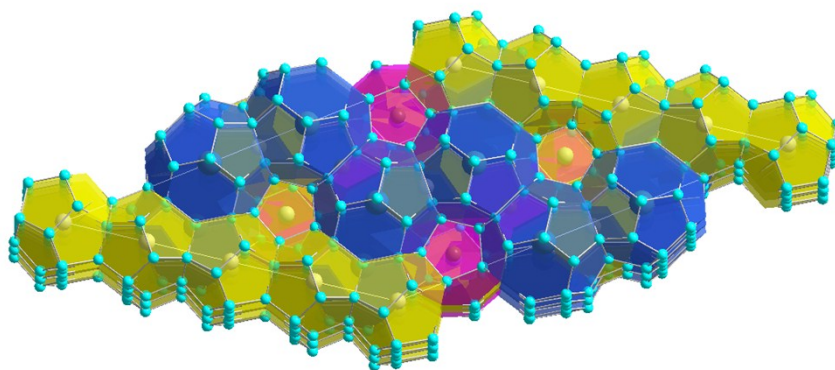


Fig. Theoretical calculation structure model of  $\text{Cs}_8\text{Na}_{10}\text{Tl}_6\text{Ge}_{136}$  in  $C2/m$  space group with  $a = b = 21.9114 \text{ \AA}$ ,  $c = 26.8359 \text{ \AA}$  and  $\beta = 144.7356^\circ$ : Na/Tl lie in the center of yellow/pink 20-vertex pentagonal dodecahedra  $[5^{12}]$  and Cs reside in the center of blue 28-vertex hexakaidecahedra  $[5^{12}6^4]$  built by Ge.