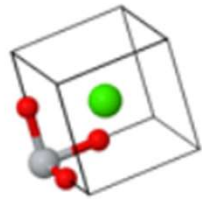


Crystal structure / Crystal physics

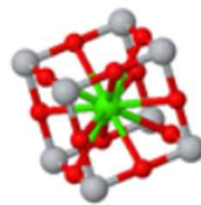
Asymmetric unit



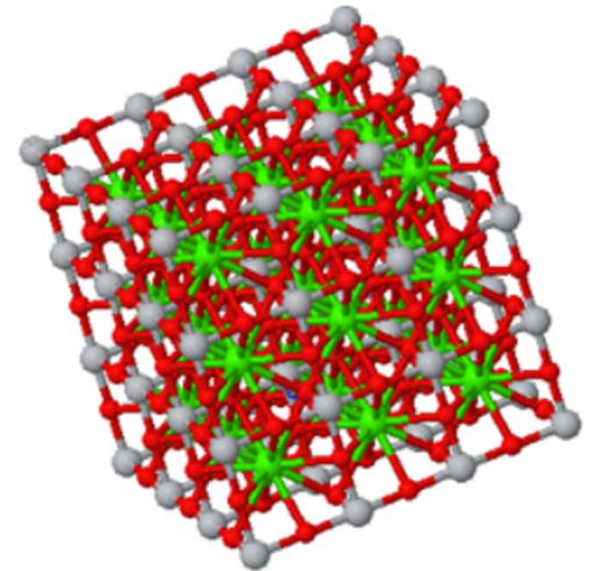
Asymmetric unit



Primitive unit cell



Conventional unit cell



Crystal

CIF files and programs to visualize crystal structures

Crystal structure data is often stored in a [CIF file](#). This is a text file that contains the asymmetric unit of the crystal, the symmetries of the space group, and a reference to the source where the data was first published. It is important to check the publication to see the conditions used during the experiment. Some experiments are performed at high temperatures or high pressures where the crystal structure can be different than at room temperature and ambient pressure. The links below will display a crystal structure and its corresponding CIF file.

Simple Cubic, Polonium Po $Pm\bar{3}m$ #221
Face-centered Cubic (fcc) $Fm\bar{3}m$ #225
Body-centered Cubic (bcc) $Im\bar{3}m$ #229
Hexagonal, Boron nitride BN #194
Hexagonal Close Packed (hcp) $P63/mmc$ #194
Perovskite, Calcium titanate $CaTiO_3$ (perovskite) $Pm\bar{3}m$ #221
Caesium chloride $CsCl$ $Pm\bar{3}m$ #221
Rocksalt $NaCl$ $Fm\bar{3}m$ #225
Zincblende #216
Wurtzite #186
Diamond (C) #227
 β -Sn #141
Graphite C $P63mc$ #186

Sucrose $P21$ #4
Magnetite Fe_3O_4 $Fd\bar{3}m$ #227
Cementite Fe_3C #62
Copper oxide CO (Tenorite) #15
Pyrite FeS_2 #205
Rutile TiO_2 #136
Spinel $MgAl_2O_4$ #227
 Sr_2FeMoO_6 (double perovskite) $I4/mmm$ #139
 $YBa_2Cu_3O_7$ #47
ZIF8 #1
Zinc oxide ZnO (wurtzite) $P63mc$ #186
ZnS (wurtzite) #186

Prototypes

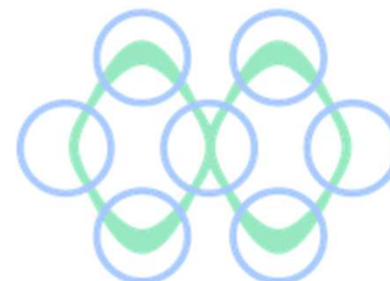
Periodic Table

Semiconductors

Ceramics



Inorganic Crystal Structure Database



Materials Project

Sodalite

From Wikipedia, the free encyclopedia

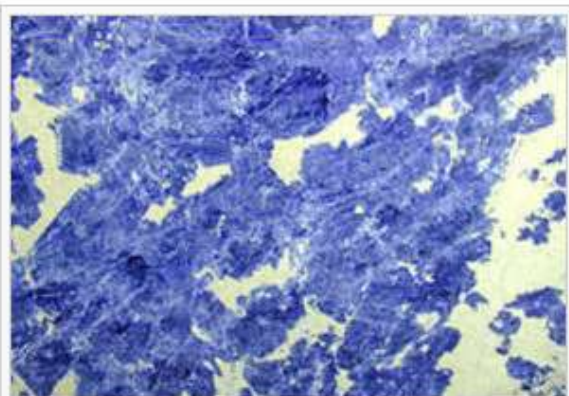
Sodalite is a rich royal blue mineral widely enjoyed as an *ornamental gemstone*. Although massive sodalite samples are opaque, crystals are usually transparent to translucent. Sodalite is a member of the sodalite group with *hauyne*, *nosean*, *lazurite* and *tugtupite*.

Discovered in 1811 in the *Ilimaussaq intrusive complex* in *Greenland*, sodalite did not become important as an ornamental stone until 1891 when vast deposits of fine material were discovered in *Ontario, Canada*.

Contents [hide]

- 1 Properties
- 2 Hackmanite
- 3 Occurrence
- 4 References

Properties [edit]



A sample of **sodalite-carbonate nephrite** from *Bolivia*, with a polished rock.

A light, relatively hard yet fragile mineral, sodalite is named after its *sodium* content; in *mineralogy* it may be classed as a *feldspathoid*. Well known for its blue color, sodalite may also be grey, yellow, green, or pink and is often mottled with white veins or patches. The more uniformly blue material is used in *jewellery*, where it is fashioned into *cabochons* and *beads*. Lesser material is more often seen as facing or inlay in

Sodalite



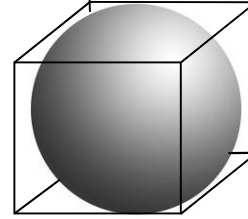
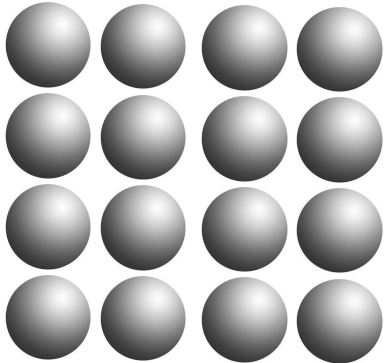
A sample of sodalite

General

Category	Tectosilicates without zeolitic H ₂ O
Formula (repeating unit)	Na ₈ (Al ₆ Si ₆ O ₂₄)Cl ₂
Strunz classification	09.FB.10
Crystal symmetry	Isometric hextetrahedral H-M symbol: $\bar{4}3m$ Space group: P $\bar{4}3n$
Unit cell	a = 8.876(6) Å; Z = 1

Identification

atomic packing density



$$\frac{\frac{4}{3} \pi (L/2)^3}{L^3} = \frac{\pi}{6} \approx 0.52$$

fcc, hcp = 0.74

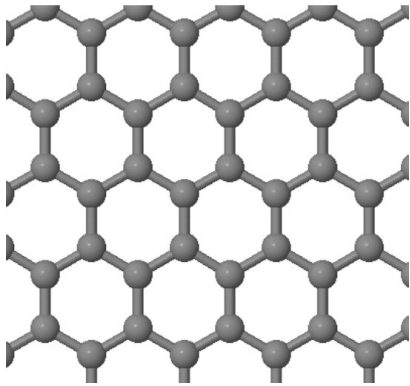
random close pack = 0.64

simple cubic = 0.52

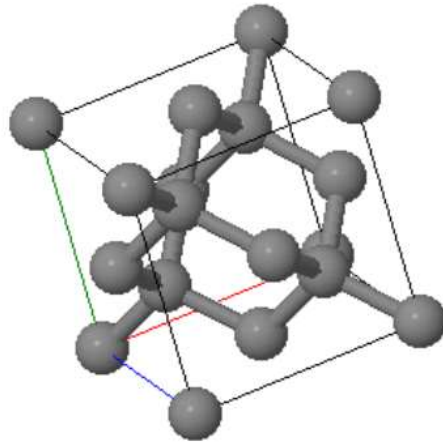
diamond = 0.34

Coordination number

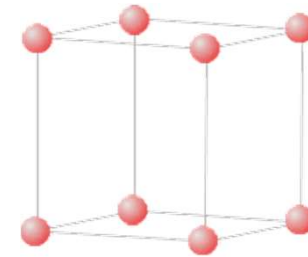
Number of nearest neighbors an atom has in a crystal



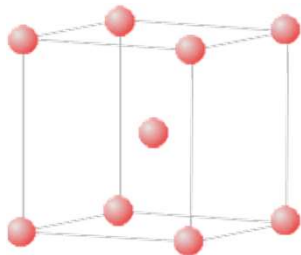
Graphene 3



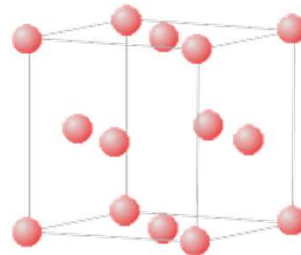
diamond 4



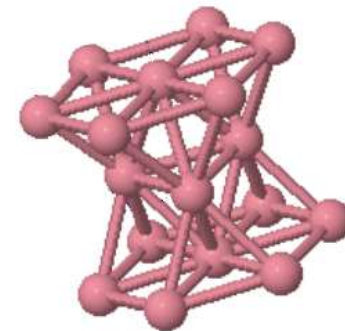
sc 6



bcc 8



fcc 12



hcp 12

Crystal physics

Crystal Physics

Crystal physics explains what effects the symmetries of the crystal have on observable quantities.

An Introduction to Crystal Physics Ervin Hartmann

<http://ww1.iucr.org/comm/cteach/pamphlets/18/index.html>

International Tables for Crystallography

<http://it.iucr.org/>

Kittel chapter 3: elastic strain

www.alnaden.ibm.com/vis/stm/atomo.html

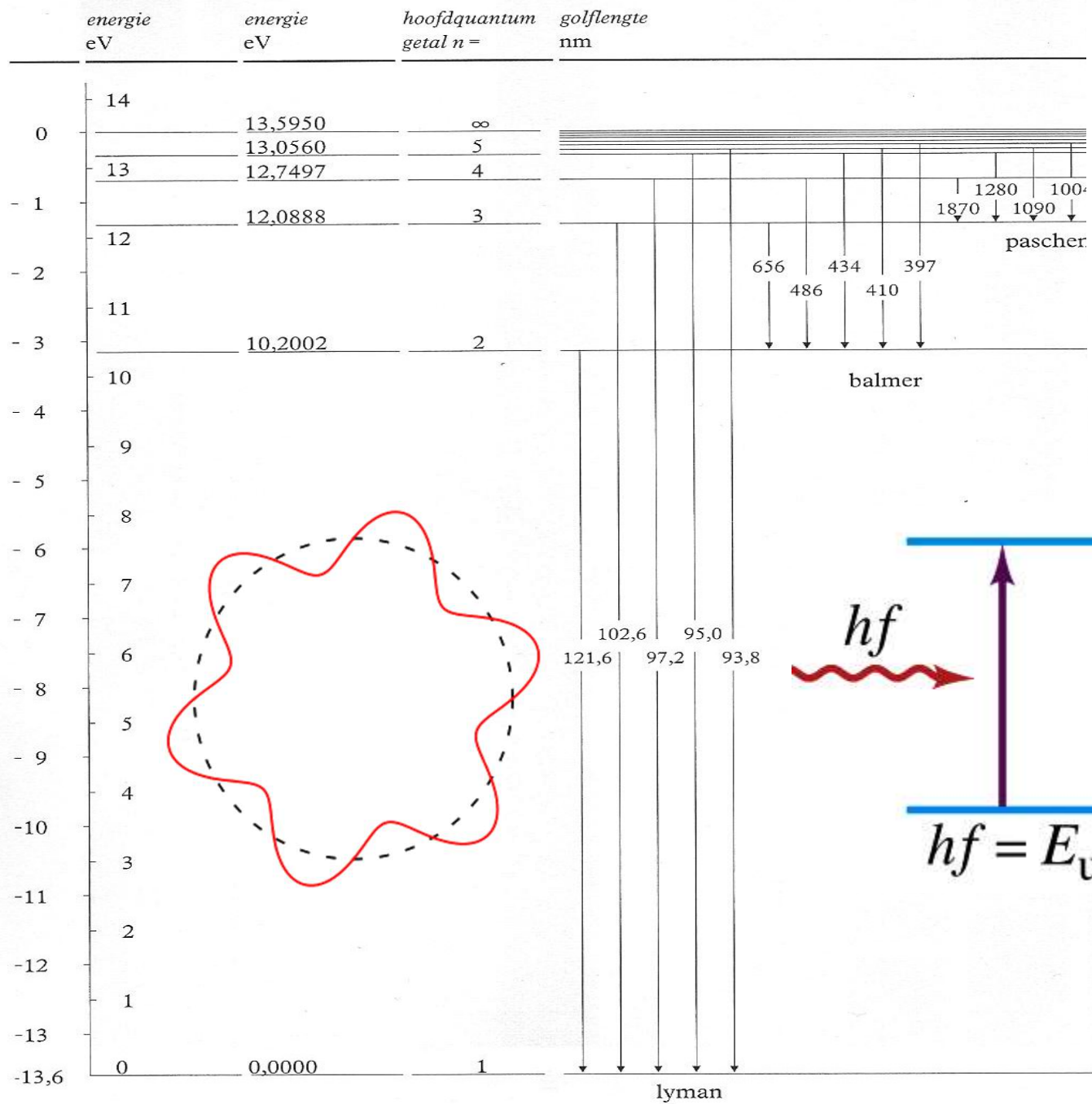
Quantum Mechanics

Everything moves like a wave but exchanges energy and momentum like a particle.

Everything moves like a wave but exchanges energy and momentum like a particle.

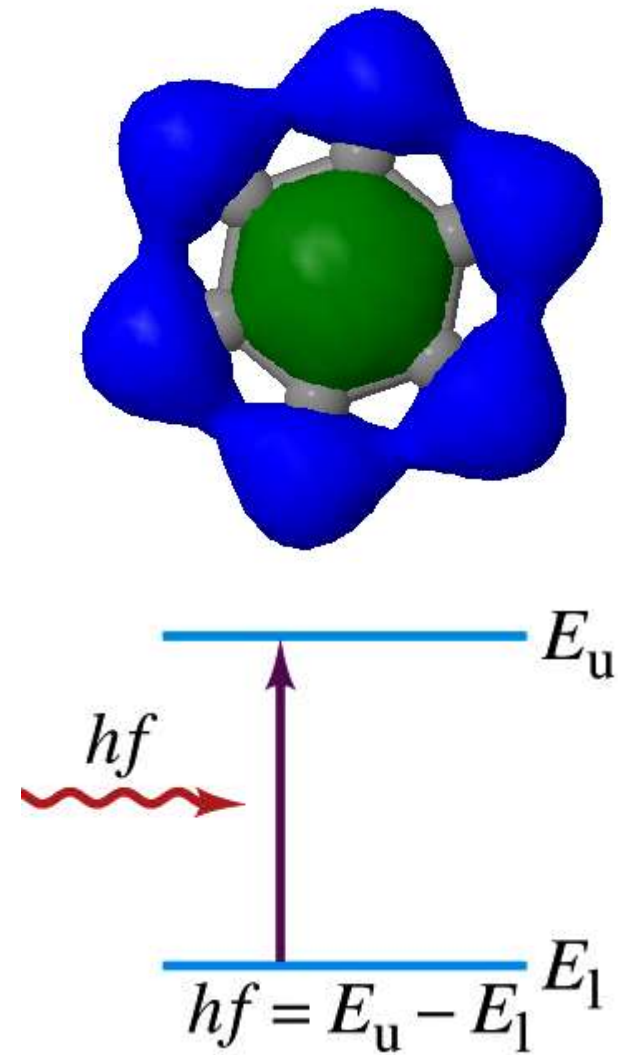
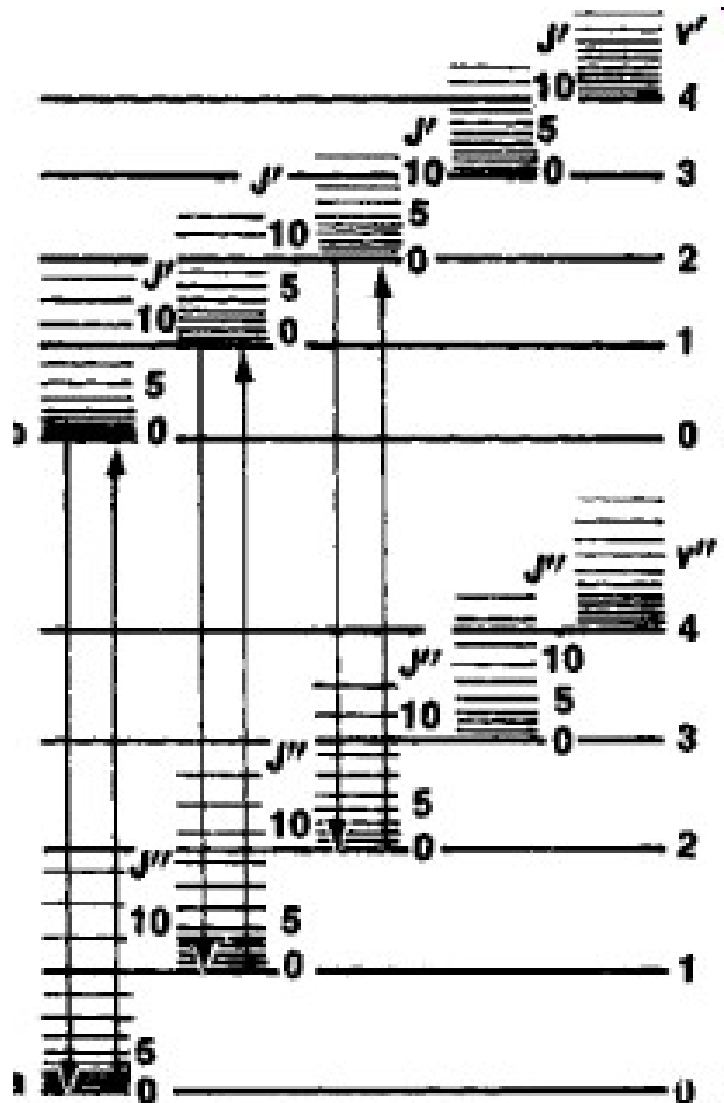


de aangegeven golflengten gelden in vacuüm



Fluorescent lamp

Molecular energy levels



Statistical Physics

Internal energy: sum over occupied electron states.

Independent variables are extrinsic quantities $U(S, M, P, \varepsilon, N)$.

$$dU = \frac{\partial U}{\partial S} dS + \frac{\partial U}{\partial \varepsilon_{ij}} d\varepsilon_{ij} + \frac{\partial U}{\partial P_k} dP_k + \frac{\partial U}{\partial M_l} dM_l$$

$$dU = TdS + \sigma_{ij}d\varepsilon_{ij} + E_k dP_k + H_l dM_l$$

Canonical ensemble: At constant temperature, make a Legendre transformation to the Helmholtz free energy.

$$F = U - TS$$

$$F(V, T, N, M, P, \varepsilon)$$

Make a Legendre transformation to the Gibbs potential $G(T, H, E, \sigma)$

$$G = U - TS - \sigma_{ij}\varepsilon_{ij} - E_k P_k - H_l M_l$$

Internal energy in an electric field

In an electric field, if the dipole moment is changed, the change of the energy is,

$$\Delta U = \vec{E} \cdot \Delta \vec{P}$$

Using Einstein notation

$$dU = E_k dP_k$$

This is part of the total derivative of U

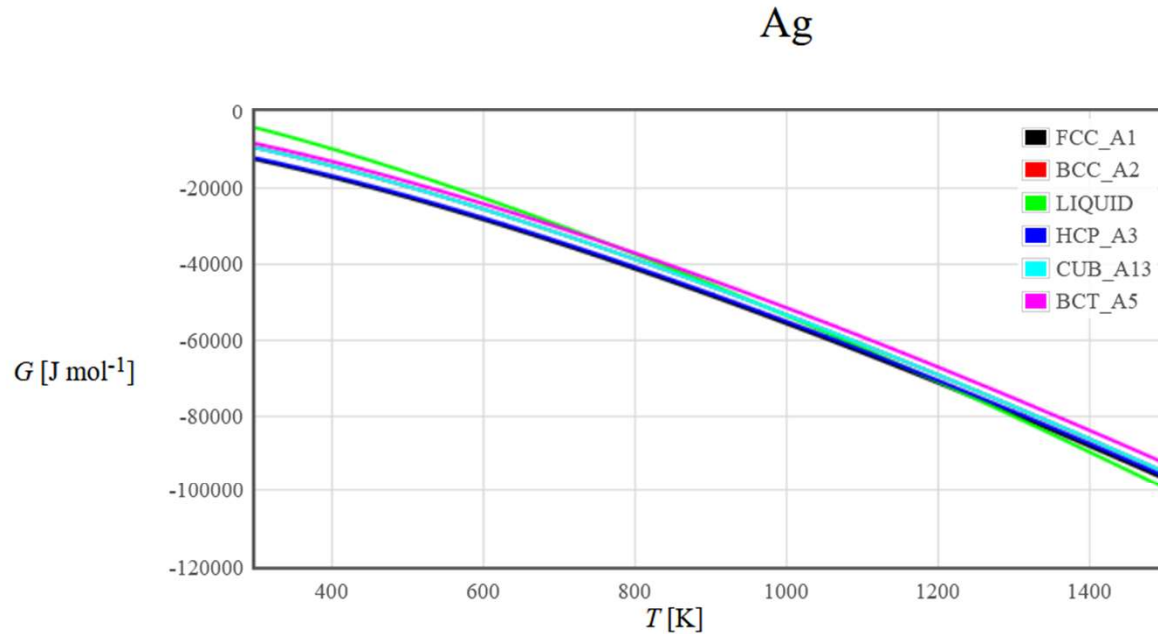
$$dU = TdS + \sigma_{ij} d\varepsilon_{ij} + E_k dP_k + H_l dM_l$$

SGTE thermodynamic data

The [Scientific Group Thermodata Europe SGTE](http://www.sgte.org) maintains [thermodynamic databanks for inorganic and metallurgical systems](http://www.sgte.org). Data from their 'pure element database' is plotted below.

Typically, experiments are performed at constant pressure p , temperature T , and number N . Under these conditions, the system will go to the minimum of the Gibbs energy $G = U + pV - TS$. Here U is the internal energy, V is the volume, and S is the entropy. The top plot is the Gibbs energy per mole.

Ag	Al	Am	As
Au	B	Ba	Be
Bi	C	Ca	Cd
Ce	Co	Cr	Cs
Cu	Dy	Er	Eu
Fe	Ga	Gd	Ge
Hf	Hg	Ho	In
Ir	K	La	Li
Lu	Mg	Mn	Mo
N	Na	Nb	Nd
Ni	Np	O	Os
P	Pa	Pb	Pd
Pr	Pt	Pu	Rb
Re	Rh	Ru	S
Sb	Sc	Se	Si
Sm	Sn	Sr	Ta
Tb	Tc	Te	Th
Ti	Tl	Tm	U
V	W	Y	Yb
Zn	Zr		



Since the Gibbs energies of the different phases fall almost on top of each other, it is convenient to plot them relative to the phase that has the lowest Gibbs energy at low temperature.

Gibbs free energy

$$G = U - TS - \sigma_{ij}\varepsilon_{ij} - E_k P_k - H_l M_l$$

$$dG = dU - TdS - SdT - \sigma_{ij}d\varepsilon_{ij} - \varepsilon_{ij}d\sigma_{ij} - E_k dP_k - P_k dE_k - H_l dM_l - M_l dH_l$$

$$dU = TdS + \sigma_{ij}d\varepsilon_{ij} + E_k dP_k + H_l dM_l$$

$$dG = -SdT - \varepsilon_{ij}d\sigma_{ij} - P_k dE_k - M_l dH_l$$

$$\text{total derivative: } dG = \left(\frac{\partial G}{\partial T}\right)dT + \left(\frac{\partial G}{\partial \sigma_{ij}}\right)d\sigma_{ij} + \left(\frac{\partial G}{\partial E_k}\right)dE_k + \left(\frac{\partial G}{\partial H_l}\right)dH_l$$

$$\left(\frac{\partial G}{\partial \sigma_{ij}}\right) = -\varepsilon_{ij} \quad \left(\frac{\partial G}{\partial E_k}\right) = -P_k$$

$$\left(\frac{\partial G}{\partial H_l}\right) = -M_l \quad \left(\frac{\partial G}{\partial T}\right) = -S$$

$$\begin{aligned}
d\epsilon_{ij} &= \left(\frac{\partial \epsilon_{ij}}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial \epsilon_{ij}}{\partial E_k}\right) dE_k + \left(\frac{\partial \epsilon_{ij}}{\partial H_l}\right) dH_l + \left(\frac{\partial \epsilon_{ij}}{\partial T}\right) dT \\
dP_i &= \left(\frac{\partial P_i}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial P_i}{\partial E_k}\right) dE_k + \left(\frac{\partial P_i}{\partial H_l}\right) dH_l + \left(\frac{\partial P_i}{\partial T}\right) dT \\
dM_i &= \left(\frac{\partial M_i}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial M_i}{\partial E_k}\right) dE_k + \left(\frac{\partial M_i}{\partial H_l}\right) dH_l + \left(\frac{\partial M_i}{\partial T}\right) dT \\
dS &= \left(\frac{\partial S}{\partial \sigma_{kl}}\right) d\sigma_{kl} + \left(\frac{\partial S}{\partial E_k}\right) dE_k + \left(\frac{\partial S}{\partial H_l}\right) dH_l + \left(\frac{\partial S}{\partial T}\right) dT
\end{aligned}$$

1. Elastic deformation.
2. Reciprocal (or converse) piezo-electric effect.
3. Reciprocal (or converse) piezo-magnetic effect.
4. Thermal dilatation.
5. Piezo-electric effect.
6. Electric polarization.
7. Magneto-electric polarization.
8. Pyroelectricity.
9. Piezo-magnetic effect.
10. Reciprocal (or converse) magneto-electric polarization.
11. Magnetic polarization.
12. Pyromagnetism.
13. Piezo-caloric effect.
14. Electro-caloric effect.
15. Magneto-caloric effect.
16. Heat transmission.