

Lithium data

Quantities that use the Mathematica “Quantity” functionality have the first letter in *script*.

```
celsiusToKelvin =
  Quantity[0., "DegreesCelsius"] // UnitConvert // QuantityMagnitude;
kb = UnitConvert[Quantity["BoltzmannConstant"], "Joules" / "Kelvins"];
kb = kb // UnitConvert // QuantityMagnitude;
```

The atomic weight of natural lithium varies from source to source, such that IUPAC [1] does not provide one number for a ‘standard atomic weight’ as it does for most elements, rather it gives the range [6.938, 6.997]. It does provide a ‘conventional atomic weight’ of Li of 6.94, “For users needing an atomic-weight value for an unspecified sample with disregard to the uncertainty, such as for trade and commerce”. In further studies we will use 6.94, but here the values 6.941 and 6.9 are retained for consistency.

[1] Meija, Juris, Tyler B. Coplen, Michael Berglund, Willi A. Brand, Paul De Bièvre, Manfred Gröning, Norman E. Holden, et al. “Atomic Weights of the Elements 2013 (IUPAC Technical Report).” Pure and Applied Chemistry 88, no. 3 (January 1, 2016). <https://doi.org/10.1515/pac-2015-0305>.

```
mLi = 6.941 Quantity["AtomicMassUnit"];
mLi = mLi // UnitConvert // QuantityMagnitude; (* in kg *)
```

This single value for the latent heat of lithium, 147 kJ/mol, was curated by Mathematica. The literature, such as from Golubchikov, below, gives latent heat values as a function of temperature. This value is consistent with Golubchikov’s values to within 5% between the melting point of lithium up to 1000K.

```
#Li = Quantity[147 \times 10^3, "Joules" / "Moles"] (* latent heat of vaporization,
Quantity[6.9 \times 10^-3, "Kilograms" / "Moles"]
from http://www.periodictable.com/Elements/003/data.html *);
lLi = #Li // QuantityMagnitude;
```

Vapor pressure of lithium, in Pascals, as a function of temperature. This value, from [3], is a truncated version of the best fit given in [2]. Future work will use [2].

[2] Browning, P, and P. E. Potter. “Section 6.2: Assessment of the Experimentally Determined Vapour Pressures of the Liquid Alkali Metals.” In Handbook of Thermodynamic and Transport Properties of Alkali Metals, edited by R.W. Ohse, 349–58. Oxford: Blackwell Scientific Publications, 1985.

[3] Section 8.1.2 of http://www.fusion.ucla.edu/APEX/interim_report/chapter8full2.pdf Chapter 8: Data base for liquid breeders and coolants. Contributors: Kai Sze, Ralph Moir, Steve Zinkle.

```
pLi[TK_] := Exp[26.89 - 18880 / TK - 0.4942 Log[TK]];
```

Here, the density of lithium vapor is calculated according to the ideal gas law, assuming that Li is entirely a gas of monomers.

```
pLi[TK_] := Quantity[pLi[TK], "Pascals"];
pLi[TK_Quantity] := Quantity[pLi[QuantityMagnitude[TK]], "Pascals"];

neqLi[TC_] := UnitConvert[pLi[TC + celsiusToKelvin] /
    (kb Quantity[(TC + celsiusToKelvin), "Kelvins"]), "Meters"^-3];
neqLi[TK_Quantity] := UnitConvert[pLi[TK] / (kb TK)];

neqLi[TC_] := neqLi[TC] // UnitConvert // QuantityMagnitude;
```

The Hertz-Knudsen one-way flux through a surface area.

```
In[114]:= (* Hertz-Knudsen-Langmuir vapor flux*)
rLi[TK_Quantity] := neqLi[TK] Sqrt[kb TK / (2 \[Pi] mLi)] // UnitConvert;
rLi[TK_] := rLi[Quantity[TK, "Kelvins"]]
```

The flux of latent heat through a surface area.

```
(* Latent heat flux through a surface at some density and temperature *)
rLi[n_, TK_] := rLi mLi n Sqrt[kb TK / (2 \[Pi] mLi)] // UnitConvert
```

Alternate Li data

Vapor pressure of lithium.

Vapor pressure of lithium, as reported in [4].

[4] Golubchikov, L. G., V. A. Evtikhin, I. E. Lyublinski, V. I. Pistunovich, I. N. Potapov, and A. N. Chumanov. "Development of a Liquid-Metal Fusion Reactor Divertor with a Capillary-Pore System." Journal of Nuclear Materials 233 (1996): 667–672.

```
pLiGolub[TK_] := 10^(12.4037 - 8283.1 / TK - 0.7081 Log10[TK])
```

Notes: Golubchikov's table also gives values for 200, 600, and 1200°C, = {1.4 10⁻⁶, 14.8, and 42650 Pa}. They don't seem to match with the formula.

Latent heat of evaporation, as a function of temperature.

From [4].

$$\text{TaLiTGolub[TK_] := } 2.4525 \times 10^7 - 2967.14 (TK + 273) - 0.1762 (TK + 273)^2;$$