12th August 2016
Note added after first publication: This Supplementary Information file is provided in addition to those published on 12th November 2015, and clarifies the parameterisation presented in the main article.

Clarification of parameterisation

The general form of the parameterisation includes several values that are themselves functions of temperature and pressure.

$$\begin{aligned}\mu_{\mathrm{S}}(T,P) = &\frac{1}{2}\left(\operatorname{erfc}\left(\frac{T-T_{tr}}{w}\right)\right)\frac{\mu_{\mathrm{S8}}}{8}\\ &+\frac{1}{2}\left(\operatorname{erf}\left(\frac{T-T_{tr}}{w}\right)+1\right)\frac{\mu_{\mathrm{S2}}}{2}\\ &-a\exp\left(-\frac{(T-(T_{tr}-b)))^2}{2c^2}\right)\end{aligned}$$

where T_{tr} and a are represented by the polynomials in $\log_{10}(P/\mathrm{Pa})$

$$\begin{aligned}T_{tr} &= \sum_i x_{Ttr,i}\left(\log_{10}\left(\frac{P}{\mathrm{Pa}}\right)\right)^i\\ a &= a_0 + a_1\log_{10}\left(\frac{P}{\mathrm{Pa}}\right) + a_2\left(\log_{10}\left(\frac{P}{\mathrm{Pa}}\right)\right)^2,\end{aligned}$$

and μ_{S8}, μ_{S2} are pressure-corrected polynomials in T

$$\begin{aligned}\mu_{\mathrm{S8}} &= \sum_i x_{\mathrm{S8},i}T^i + kT\ln\frac{P}{P_{\mathrm{ref}}},\\ \mu_{\mathrm{S2}} &= \sum_i x_{\mathrm{S2},i}T^i + kT\ln\frac{P}{P_{\mathrm{ref}}}\end{aligned}$$

where P_{ref} is 10^5 Pa.

Tabulated values are given below in two systems of units. In all cases the group $\frac{P}{\mathrm{Pa}}$ is equal to the pressure in Pascals. If calculating the properties for a basis of one mole of S atoms (i.e. in J mol^{-1}) then k is the gas constant $R = 8.314$ J mol^{-1} K^{-1}. For a basis of one atom k should be set to the Boltzmann constant $k_B = 8.617$E-5 eV K^{-1}.

Parameter	Value	units	Value	units
$x_{S8,0}$	7.352E+04	J mol^{-1}	7.620E-01	eV atom^{-1}
$x_{S8,1}$	-2.370E+02	J mol^{-1} / K	-2.457E-03	eV atom^{-1} / K
$x_{S8,2}$	-3.871E-01	J mol^{-1} / K^2	-4.012E-06	eV atom^{-1} / K^2
$x_{S8,3}$	1.744E-04	J mol^{-1} / K^3	1.808E-09	eV atom^{-1} / K^3
$x_{S8,4}$	-3.676E-08	J mol^{-1} / K^4	-3.810E-13	eV atom^{-1} / K^4
$x_{S2,0}$	1.165E+05	J mol^{-1}	1.207E+00	eV atom^{-1}
$x_{S2,1}$	-1.783E+02	J mol^{-1} / K	-1.848E-03	eV atom^{-1} / K
$x_{S2,2}$	-8.265E-02	J mol^{-1} / K^2	-8.566E-07	eV atom^{-1} / K^2
$x_{S2,3}$	3.860E-05	J mol^{-1} / K^3	4.001E-10	eV atom^{-1} / K^3
$x_{S2,4}$	-8.350E-09	J mol^{-1} / K^4	-8.654E-14	eV atom^{-1} / K^4
$x_{Ttr,0}$	5.077E+02	K		
$x_{Ttr,1}$	7.272E+01	K		
$x_{Ttr,2}$	-8.295E+00	K		
$x_{Ttr,3}$	1.828E+00	K		
a_0	1.414E+03	J mol^{-1}	1.465E-02	eV atom^{-1}
a_1	-2.041E+02	J mol^{-1}	-2.115E-03	eV atom^{-1}
a_2	6.663E+01	J mol^{-1}	6.905E-04	eV atom^{-1}
b	10	K		
c	80	K		
w	100	K		