Thermodynamics of Ionized Argon

Physical constants

In[249]:=
```
Ru = 8314.472; MWar = 39.948; MWarII = 39.94745; MWe = 0.000548579903;
```

Units

In[250]:=
```
MJ = 10^6; kJ = 10^3; bar = 10^5;
```

Reference state

In[251]:=
```
pref = 1 bar;
```

Enthalpy of formation

Source: NASA-TP-2002-211556

https://ntrs.nasa.gov/api/citations/20020085330/downloads/20020085330.pdf

Argon (ArI) [units: J/kmol]

In[252]:= $h_{fAr} = 0.;$

Ionized Argon (ArII) [units: J/kmol]

Note: “All reference elements and **the reference species electron gas** have assigned enthalpy values, Ho(298.15), **equal to zero**,” so this value include the energy of ionization of Argon and the freed electron.

In[253]:= $h_{fArII} = 1\,526\,778.407;$

In[254]:= $h_{fe} = 0;$

NASA fits for c_p

Source: NASA-TP-2002-211556

https://ntrs.nasa.gov/api/citations/20020085330/downloads/20020085330.pdf

NASA fits for Argon (ArI)

In[255]:=

$$a_{1\,Ara} = 0.;\quad a_{2\,Ara} = 0.;\quad a_{3\,Ara} = 2.5;\quad a_{4\,Ara} = 0.;\quad a_{5\,Ara} = 0.;\quad a_{6\,Ara} = 0.;\quad a_{7\,Ara} = 0.;$$
$$b_{1\,Ara} = -7.453750000\times10^{2};\quad b_{2\,Ara} = 4.379674910;$$

In[256]:=

$$a_{1\,Arb} = 2.010538475\times10^{1};\quad a_{2\,Arb} = -5.992661070\times10^{-2};\quad a_{3\,Arb} = 2.500069401;$$
$$a_{4\,Arb} = -3.992141160\times10^{-8};\quad a_{5\,Arb} = 1.205272140\times10^{-11};\quad a_{6\,Arb} = -1.819015576\times10^{-15};$$
$$a_{7\,Arb} = 1.078576636\times10^{-19};\quad b_{1\,Arb} = -7.449939610\times10^{2};\quad b_{2\,Arb} = 4.379180110;$$

In[257]:=

$$a_{1\,Arc} = -9.951265080\times10^{8};\quad a_{2\,Arc} = 6.458887260\times10^{5};\quad a_{3\,Arc} = -1.675894697\times10^{2};$$
$$a_{4\,Arc} = 2.319933363\times10^{-2};\quad a_{5\,Arc} = -1.721080911\times10^{-6};\quad a_{6\,Arc} = 6.531938460\times10^{-11};$$
$$a_{7\,Arc} = -9.740147729\times10^{-16};\quad b_{1\,Arc} = -5.078300340\times10^{6};\quad b_{2\,Arc} = 1.465298484\times10^{3};$$

In[262]:=

$$cp_{Ar}[T\_] := Ru * Which[$$
$$T \le 1000,$$
$$a_{1\,Ara}\,T^{-2} + a_{2\,Ara}\,T^{-1} + a_{3\,Ara} + a_{4\,Ara}\,T + a_{5\,Ara}\,T^{2} + a_{6\,Ara}\,T^{3} + a_{7\,Ara}\,T^{4},$$
$$1000 < T \le 6000,$$
$$a_{1\,Arb}\,T^{-2} + a_{2\,Arb}\,T^{-1} + a_{3\,Arb} + a_{4\,Arb}\,T + a_{5\,Arb}\,T^{2} + a_{6\,Arb}\,T^{3} + a_{7\,Arb}\,T^{4},$$
$$T > 6000,$$
$$a_{1\,Arc}\,T^{-2} + a_{2\,Arc}\,T^{-1} + a_{3\,Arc} + a_{4\,Arc}\,T + a_{5\,Arc}\,T^{2} + a_{6\,Arc}\,T^{3} + a_{7\,Arc}\,T^{4}]$$

In[263]:= $h_{Ar}[T\_] := Ru\,T * \text{Which}\Big[$

$T \le 1000,$

$-a_{1\,Ara} T^{-2} + a_{2\,Ara} \text{Log}[T]\, T^{-1} + a_{3\,Ara} + a_{4\,Ara} \frac{T}{2} + a_{5\,Ara} \frac{T^2}{3} + a_{6\,Ara} \frac{T^3}{4} + a_{7\,Ara} \frac{T^4}{5} + b_{1\,Ara} T^{-1},$

$1000 < T \le 6000,$

$-a_{1\,Arb} T^{-2} + a_{2\,Arb} \text{Log}[T]\, T^{-1} + a_{3\,Arb} + a_{4\,Arb} \frac{T}{2} + a_{5\,Arb} \frac{T^2}{3} + a_{6\,Arb} \frac{T^3}{4} + a_{7\,Arb} \frac{T^4}{5} + b_{1\,Arb} T^{-1},$

$T > 6000,$

$-a_{1\,Arc} T^{-2} + a_{2\,Arc} \text{Log}[T]\, T^{-1} + a_{3\,Arc} + a_{4\,Arc} \frac{T}{2} + a_{5\,Arc} \frac{T^2}{3} + a_{6\,Arc} \frac{T^3}{4} + a_{7\,Arc} \frac{T^4}{5} + b_{1\,Arc} T^{-1}\Big]$

In[264]:= $s_{Ar}[T\_] := Ru * \text{Which}\Big[$

$T \le 1000,$

$-a_{1\,Ara} \frac{T^{-2}}{2} - a_{2\,Ara} T^{-1} + a_{3\,Ara} \text{Log}[T] + a_{4\,Ara} T + a_{5\,Ara} \frac{T^2}{2} + a_{6\,Ara} \frac{T^3}{3} + a_{7\,Ara} \frac{T^4}{4} + b_{2\,Ara},$

$1000 < T \le 6000,$

$-a_{1\,Arb} \frac{T^{-2}}{2} - a_{2\,Arb} T^{-1} + a_{3\,Arb} \text{Log}[T] + a_{4\,Arb} T + a_{5\,Arb} \frac{T^2}{2} + a_{6\,Arb} \frac{T^3}{3} + a_{7\,Arb} \frac{T^4}{4} + b_{2\,Arb},$

$T > 6000,$

$-a_{1\,Arc} \frac{T^{-2}}{2} - a_{2\,Arc} T^{-1} + a_{3\,Arc} \text{Log}[T] + a_{4\,Arc} T + a_{5\,Arc} \frac{T^2}{2} + a_{6\,Arc} \frac{T^3}{3} + a_{7\,Arc} \frac{T^4}{4} + b_{2\,Arc}\Big]$

In[265]:= $g_{Ar}{}^{*}[T\_] := h_{Ar}[T] - T\, s_{Ar}[T]$

In[266]:= $g_{Ar}[T\_, p\_, n\_, ntot\_] := g_{Ar}{}^{*}[T] + Ru\,T\,\text{Log}[n] - Ru\,T\,\text{Log}[ntot] + Ru\,T\,\text{Log}\left[\frac{p}{pref}\right]$

In[267]:= $u_{Ar}[T\_] := h_{Ar}[T] - Ru\,T$

In[268]:= $u_{Ar}[3000] - u_{Ar}[300]$

Out[268]= 3.36736×10^{7}

Ar properties on per kmol basis

In[269]:=
```
TableForm[Table[{i * 1000, gAr[1000 * i, 0.1 bar, 1 , 1] / MJ, gAr[1000 * i, 1 bar, 1 , 1] / MJ,
   gAr[1000 * i, 10 bar, 1 , 1] / MJ}, {i, 1, 20}], TableHeadings →
  {None, {"Temp (K)", "g (MJ/kmol) 0.1 bar", "g (MJ/kmol) 1 bar", "g (MJ/kmol) 10 bar"}}]
```

Out[269]//TableForm=

Temp (K)	g (MJ/kmol) 0.1 bar	g (MJ/kmol) 1 bar	g (MJ/kmol) 10 bar
1000	-184.557	-165.412	-146.267
2000	-391.731	-353.442	-315.152
3000	-609.783	-552.348	-494.914
4000	-834.897	-758.318	-681.739
5000	-1065.26	-969.539	-873.816
6000	-1299.82	-1184.95	-1070.08
7000	-1537.85	-1403.84	-1269.82
8000	-1778.86	-1625.71	-1472.55
9000	-2022.48	-1850.18	-1677.88
10000	-2268.42	-2076.97	-1885.52
11000	-2516.45	-2305.85	-2095.26
12000	-2766.39	-2536.65	-2306.91
13000	-3018.1	-2769.22	-2520.34
14000	-3271.5	-3003.47	-2735.44
15000	-3526.53	-3239.36	-2952.19
16000	-3783.19	-3476.87	-3170.56
17000	-4041.52	-3716.05	-3390.59
18000	-4301.56	-3956.96	-3612.35
19000	-4563.4	-4199.65	-3835.9
20000	-4827.08	-4444.18	-4061.29

Ar properties on per kg basis

In[270]:=
```
TableForm[Table[
  {i * 1000, gAr[1000 * i, 0.1 bar, 1 , 1] / MWar / kJ, gAr[1000 * i, 1 bar, 1 , 1] / MWar / kJ,
   gAr[1000 * i, 10 bar, 1 , 1] / MWar / kJ}, {i, 1, 20}], TableHeadings →
  {None, {"Temp (K)", "g (kJ/kg) 0.1 bar", "g (kJ/kg) 1 bar", "g (kJ/kg) 10 bar"}}]
```

Out[270]//TableForm=

Temp (K)	g (kJ/kg) 0.1 bar	g (kJ/kg) 1 bar	g (kJ/kg) 10 bar
1000	-4619.92	-4140.68	-3661.43
2000	-9806.03	-8847.55	-7889.06
3000	-15 264.4	-13 826.7	-12 389.
4000	-20 899.6	-18 982.6	-17 065.7
5000	-26 666.3	-24 270.	-21 873.8
6000	-32 537.7	-29 662.2	-26 786.8
7000	-38 496.3	-35 141.6	-31 786.9
8000	-44 529.5	-40 695.6	-36 861.6
9000	-50 627.9	-46 314.7	-42 001.5
10 000	-56 784.3	-51 991.8	-47 199.4
11 000	-62 993.1	-57 721.4	-52 449.7
12 000	-69 249.7	-63 498.8	-57 747.9
13 000	-75 550.8	-69 320.6	-63 090.5
14 000	-81 893.9	-75 184.5	-68 475.1
15 000	-88 278.	-81 089.3	-73 900.7
16 000	-94 702.9	-87 035.	-79 367.1
17 000	-101 169.	-93 022.3	-84 875.2
18 000	-107 679.	-99 052.7	-90 426.4
19 000	-114 234.	-105 128.	-96 022.3
20 000	-120 834.	-111 249.	-101 664.

NASA fits for Argon (ArII)

In[271]:=

$a_{1\,ArIIa} = -5.731209170 \times 10^{+4};$

$a_{2\,ArIIa} = 7.930791470 \times 10^{+2};$

$a_{3\,ArIIa} = -1.717121217;$

$a_{4\,ArIIa} = 1.044184018 \times 10^{-2};$

$a_{5\,ArIIa} = -1.180207501 \times 10^{-5};$

$a_{6\,ArIIa} = 6.528134780 \times 10^{-9};$

$a_{7\,ArIIa} = -1.447558130 \times 10^{-12};$

$b_{1\,ArIIa} = 1.790572230 \times 10^{+5};$

$b_{2\,ArIIa} = 2.949150950 \times 10^{+1};$

In[272]:=
$$a_{1\,ArIIb} = -3.835965400\times 10^{+5};$$
$$a_{2\,ArIIb} = 8.162019700\times 10^{+2};$$
$$a_{3\,ArIIb} = 2.301342628;$$
$$a_{4\,ArIIb} = -4.952983770\times 10^{-6};$$
$$a_{5\,ArIIb} = 1.205108477\times 10^{-8};$$
$$a_{6\,ArIIb} = -2.185050286\times 10^{-12};$$
$$a_{7\,ArIIb} = 1.265493898\times 10^{-16};$$
$$b_{1\,ArIIb} = 1.771811455\times 10^{+5};$$
$$b_{2\,ArIIb} = 7.947507480;$$

In[281]:=
$$a_{1\,ArIIc} = 1.006884827\times 10^{7};$$
$$a_{2\,ArIIc} = -6.624361280\times 10^{+3};$$
$$a_{3\,ArIIc} = 4.446908200;$$
$$a_{4\,ArIIc} = -3.017567664\times 10^{-4};$$
$$a_{5\,ArIIc} = 2.612882069\times 10^{-8};$$
$$a_{6\,ArIIc} = -1.201637769\times 10^{-12};$$
$$a_{7\,ArIIc} = 2.299206903\times 10^{-17};$$
$$b_{1\,ArIIc} = 2.349504137\times 10^{+5};$$
$$b_{2\,ArIIc} = -1.032262257\times 10^{+1};$$

In[290]:=
$$cp_{ArII}[T\_] := Ru * Which\Big[$$
$$T \le 1000,$$
$$a_{1\,ArIIa}\,T^{-2} + a_{2\,ArIIa}\,T^{-1} + a_{3\,ArIIa} + a_{4\,ArIIa}\,T + a_{5\,ArIIa}\,T^{2} + a_{6\,ArIIa}\,T^{3} + a_{7\,ArIIa}\,T^{4},$$
$$1000 < T \le 6000,$$
$$a_{1\,ArIIb}\,T^{-2} + a_{2\,ArIIb}\,T^{-1} + a_{3\,ArIIb} + a_{4\,ArIIb}\,T + a_{5\,ArIIb}\,T^{2} + a_{6\,ArIIb}\,T^{3} + a_{7\,ArIIb}\,T^{4},$$
$$T > 6000,$$
$$a_{1\,ArIIc}\,T^{-2} + a_{2\,ArIIc}\,T^{-1} + a_{3\,ArIIc} + a_{4\,ArIIc}\,T + a_{5\,ArIIc}\,T^{2} + a_{6\,ArIIc}\,T^{3} + a_{7\,ArIIc}\,T^{4}\Big]$$

In[291]:=
$$h_{ArII}[T\_] := Ru\,T * Which\Big[$$
$$T \le 1000,$$
$$-a_{1\,ArIIa}\,T^{-2} + a_{2\,ArIIa}\,Log[T]\,T^{-1}$$
$$+ a_{3\,ArIIa} + a_{4\,ArIIa}\frac{T}{2} + a_{5\,ArIIa}\frac{T^{2}}{3} + a_{6\,ArIIa}\frac{T^{3}}{4} + a_{7\,ArIIa}\frac{T^{4}}{5} + b_{1\,ArIIa}\,T^{-1},$$
$$1000 < T \le 6000,$$
$$-a_{1\,ArIIb}\,T^{-2} + a_{2\,ArIIb}\,Log[T]\,T^{-1} +$$
$$a_{3\,ArIIb} + a_{4\,ArIIb}\frac{T}{2} + a_{5\,ArIIb}\frac{T^{2}}{3} + a_{6\,ArIIb}\frac{T^{3}}{4} + a_{7\,ArIIb}\frac{T^{4}}{5} + b_{1\,ArIIb}\,T^{-1},$$
$$T > 6000,$$
$$-a_{1\,ArIIc}\,T^{-2} + a_{2\,ArIIc}\,Log[T]\,T^{-1} +$$
$$a_{3\,ArIIc} + a_{4\,ArIIc}\frac{T}{2} + a_{5\,ArIIc}\frac{T^{2}}{3} + a_{6\,ArIIc}\frac{T^{3}}{4} + a_{7\,ArIIc}\frac{T^{4}}{5} + b_{1\,ArIIc}\,T^{-1}\Big]$$

In[292]:= $s_{ArII}[T\_] := Ru * Which\Big[$

$T \le 1000,$

$-a_{1\,ArIIa}\,\frac{T^{-2}}{2} - a_{2\,ArIIa}\,T^{-1} +$

$a_{3\,ArIIa}\,Log[T] + a_{4\,ArIIa}\,T + a_{5\,ArIIa}\,\frac{T^2}{2} + a_{6\,ArIIa}\,\frac{T^3}{3} + a_{7\,ArIIa}\,\frac{T^4}{4} + b_{2\,ArIIa},$

$1000 < T \le 6000,$

$-a_{1\,ArIIb}\,\frac{T^{-2}}{2} - a_{2\,ArIIb}\,T^{-1} +$

$a_{3\,ArIIb}\,Log[T] + a_{4\,ArIIb}\,T + a_{5\,ArIIb}\,\frac{T^2}{2} + a_{6\,ArIIb}\,\frac{T^3}{3} + a_{7\,ArIIb}\,\frac{T^4}{4} + b_{2\,ArIIb},$

$T > 6000,$

$-a_{1\,ArIIc}\,\frac{T^{-2}}{2} - a_{2\,ArIIc}\,T^{-1} + a_{3\,ArIIc}\,Log[T] + a_{4\,ArIIc}\,T + a_{5\,ArIIc}\,\frac{T^2}{2} + a_{6\,ArIIc}\,\frac{T^3}{3} + a_{7\,ArIIc}\,\frac{T^4}{4} + b_{2\,ArIIc}\Big]$

In[293]:= $g_{ArII}{}^{*}[T\_] := h_{ArII}[T] - T\,s_{ArII}[T]$

In[294]:= $g_{ArII}[T\_, p\_, n\_, ntot\_] := g_{ArII}{}^{*}[T] + Ru\,T\,Log[n] - Ru\,T\,Log[ntot] + Ru\,T\,Log\left[\frac{p}{pref}\right]$

In[295]:= $u_{ArII}[T\_] := h_{ArII}[T] - Ru\,T$

In[296]:= $u_{ArII}[3000] - u_{ArII}[300]$

Out[296]= 3.71081×10^{7}

ArII properties on per kmol basis

In[297]:=
```
TableForm[
 Table[{i * 1000, gArII[1000 * i, 0.1 bar, 1 , 1] / MJ, gArII[1000 * i, 1 bar, 1 , 1] / MJ,
   gArII[1000 * i, 10 bar, 1 , 1] / MJ}, {i, 1, 20}], TableHeadings →
  {None, {"Temp (K)", "g (MJ/kmol) 0.1 bar", "g (MJ/kmol) 1 bar", "g (MJ/kmol) 10 bar"}}]
```

Out[297]//TableForm=

Temp (K)	g (MJ/kmol) 0.1 bar	g (MJ/kmol) 1 bar	g (MJ/kmol) 10 bar
1000	1330.17	1349.31	1368.46
2000	1109.25	1147.54	1185.83
3000	876.802	934.236	991.671
4000	637.066	713.645	790.224
5000	391.975	487.699	583.423
6000	142.644	257.512	372.381
7000	-110.2	23.8133	157.827
8000	-366.045	-212.886	-59.7281
9000	-624.508	-452.205	-279.902
10 000	-885.296	-693.848	-502.4
11 000	-1148.17	-937.581	-726.988
12 000	-1412.95	-1183.21	-953.474
13 000	-1679.46	-1430.58	-1181.7
14 000	-1947.58	-1679.55	-1411.53
15 000	-2217.19	-1930.02	-1642.85
16 000	-2488.19	-2181.88	-1875.56
17 000	-2760.51	-2435.04	-2109.58
18 000	-3034.06	-2689.45	-2344.84
19 000	-3308.78	-2945.03	-2581.28
20 000	-3584.64	-3201.75	-2818.85

ArII properties on per kg basis

In[298]:=
```
TableForm[Table[
  {i * 1000, g_ArII[1000 * i, 0.1 bar, 1 , 1] / MWar / kJ, g_ArII[1000 * i, 1 bar, 1 , 1] / MWar / kJ,
   g_ArII[1000 * i, 10 bar, 1 , 1] / MWar / kJ}, {i, 1, 20}], TableHeadings →
  {None, {"Temp (K)", "g (kJ/kg) 0.1 bar", "g (kJ/kg) 1 bar", "g (kJ/kg) 10 bar"}}]
```

Out[298]//TableForm=

Temp (K)	g (kJ/kg) 0.1 bar	g (kJ/kg) 1 bar	g (kJ/kg) 10 bar
1000	33 297.4	33 776.7	34 255.9
2000	27 767.3	28 725.8	29 684.2
3000	21 948.6	23 386.3	24 824.
4000	15 947.4	17 864.3	19 781.3
5000	9812.13	12 208.3	14 604.6
6000	3570.74	6446.19	9321.65
7000	-2758.59	596.106	3950.8
8000	-9163.03	-5329.09	-1495.15
9000	-15 633.	-11 319.8	-7006.66
10 000	-22 161.2	-17 368.8	-12 576.4
11 000	-28 741.7	-23 470.	-18 198.4
12 000	-35 369.7	-29 618.8	-23 867.9
13 000	-42 041.2	-35 811.1	-29 580.9
14 000	-48 752.9	-42 043.5	-35 334.1
15 000	-55 501.9	-48 313.3	-41 124.6
16 000	-62 285.8	-54 617.9	-46 950.
17 000	-69 102.5	-60 955.3	-52 808.2
18 000	-75 950.1	-67 323.8	-58 697.4
19 000	-82 827.3	-73 721.7	-64 616.1
20 000	-89 732.7	-80 147.9	-70 563.

NASA fits for electrons (e^-)

In[299]:= $a_e = 0.;$

In[300]:=
$a_{1\,ea} = 0.;$
$a_{2\,ea} = 0.;$
$a_{3\,ea} = 2.500000000;$
$a_{4\,ea} = 0.;$
$a_{5\,ea} = 0.;$
$a_{6\,ea} = 0.;$
$a_{7\,ea} = 0.;$
$b_{1\,ea} = -7.453750000 \times 10^2;$
$b_{2\,ea} = -1.172081224 \times 10^1;$

In[301]:=
```
a1 eb = 0.;
a2 eb = 0.;
a3 eb = 2.500000000; a4 eb = 0.; a5 eb = 0.;
a6 eb = 0. ;
a7 eb = 0.;
b1 eb = -7.453750000 × 10^2;
b2 eb = -1.172081224 × 10^1;
```

In[302]:=
```
a1 ec = 0.; a2 ec = 0.; a3 ec = 2.500000000;
a4 ec = 0.;
a5 ec = 0.;
a6 ec = 0.;
a7 ec = 0.;
b1 ec = -7.453750000 × 10^2;
b2 ec = -1.172081224 × 10^1;
```

In[303]:=
$cp_e[T\_] := Ru * \text{Which}[$
$T \le 1000,$
$a_{1\,ea}\, T^{-2} + a_{2\,ea}\, T^{-1} + a_{3\,ea} + a_{4\,ea}\, T + a_{5\,ea}\, T^2 + a_{6\,ea}\, T^3 + a_{7\,ea}\, T^4,$
$1000 < T \le 6000,$
$a_{1\,eb}\, T^{-2} + a_{2\,eb}\, T^{-1} + a_{3\,eb} + a_{4\,eb}\, T + a_{5\,eb}\, T^2 + a_{6\,eb}\, T^3 + a_{7\,eb}\, T^4,$
$T > 6000,$
$a_{1\,ec}\, T^{-2} + a_{2\,ec}\, T^{-1} + a_{3\,ec} + a_{4\,ec}\, T + a_{5\,ec}\, T^2 + a_{6\,ec}\, T^3 + a_{7\,ec}\, T^4]$

In[304]:=
$h_e[T\_] := Ru\, T * \text{Which}[$
$T \le 1000,$
$-a_{1\,ea}\, T^{-2} + a_{2\,ea}\, \text{Log}[T]\, T^{-1} + a_{3\,ea} + a_{4\,ea}\, \frac{T}{2} + a_{5\,ea}\, \frac{T^2}{3} + a_{6\,ea}\, \frac{T^3}{4} + a_{7\,ea}\, \frac{T^4}{5} + b_{1\,ea}\, T^{-1},$
$1000 < T \le 6000,$
$-a_{1\,eb}\, T^{-2} + a_{2\,eb}\, \text{Log}[T]\, T^{-1} + a_{3\,eb} + a_{4\,eb}\, \frac{T}{2} + a_{5\,eb}\, \frac{T^2}{3} + a_{6\,eb}\, \frac{T^3}{4} + a_{7\,eb}\, \frac{T^4}{5} + b_{1\,eb}\, T^{-1},$
$T > 6000,$
$-a_{1\,ec}\, T^{-2} + a_{2\,ec}\, \text{Log}[T]\, T^{-1} + a_{3\,ec} + a_{4\,ec}\, \frac{T}{2} + a_{5\,ec}\, \frac{T^2}{3} + a_{6\,ec}\, \frac{T^3}{4} + a_{7\,ec}\, \frac{T^4}{5} + b_{1\,ec}\, T^{-1}]$

In[305]:=
$s_e[T\_] := Ru * \text{Which}[$
$T \le 1000,$
$-a_{1\,ea}\, \frac{T^{-2}}{2} - a_{2\,ea}\, T^{-1} + a_{3\,ea}\, \text{Log}[T] + a_{4\,ea}\, T + a_{5\,ea}\, \frac{T^2}{2} + a_{6\,ea}\, \frac{T^3}{3} + a_{7\,ea}\, \frac{T^4}{4} + b_{2\,ea},$
$1000 < T \le 6000,$
$-a_{1\,eb}\, \frac{T^{-2}}{2} - a_{2\,eb}\, T^{-1} + a_{3\,eb}\, \text{Log}[T] + a_{4\,eb}\, T + a_{5\,eb}\, \frac{T^2}{2} + a_{6\,eb}\, \frac{T^3}{3} + a_{7\,eb}\, \frac{T^4}{4} + b_{2\,eb},$
$T > 6000,$
$-a_{1\,ec}\, \frac{T^{-2}}{2} - a_{2\,ec}\, T^{-1} + a_{3\,ec}\, \text{Log}[T] + a_{4\,ec}\, T + a_{5\,ec}\, \frac{T^2}{2} + a_{6\,ec}\, \frac{T^3}{3} + a_{7\,ec}\, \frac{T^4}{4} + b_{2\,ec}]$

In[306]:= $g_e{}^*[T\_] := h_e[T] - T\, s_e[T]$

In[307]:= $g_e[T\_, p\_, n\_, ntot\_] := g_e{}^*[T] + Ru\, T\, Log[n] - Ru\, T\, Log[ntot] + Ru\, T\, Log\left[\frac{p}{pref}\right]$

Solve for Equilibrium Constant

Reminder that the NASA fits enthalpy of formation, etc., "built in" to polynomial fits.

In[308]:= $\Delta G^*_{ionization}[T\_] := g_e{}^*[T] + g_{ArII}{}^*[T] - g_{Ar}{}^*[T]$

In[309]:= $K_{ionization}[T\_] := Exp\left[-\frac{\Delta G^*_{ionization}[T]}{Ru\, T}\right]$

Solve for degree of ionization analytically.

In[310]:= $Solve\left[\frac{\left(\frac{\alpha}{\alpha+1}\right)^2}{\frac{1-\alpha}{\alpha+1}}\, ppreftmp == K, \alpha\right]$

Out[310]= $\left\{\left\{\alpha \to -\frac{\sqrt{K}}{\sqrt{K + ppreftmp}}\right\}, \left\{\alpha \to \frac{\sqrt{K}}{\sqrt{K + ppreftmp}}\right\}\right\}$

Define a function for degree of ionization.

In[311]:= $\alpha[T\_, p\_] := \frac{\sqrt{K_{ionization}[T]}}{\sqrt{K_{ionization}[T] + \frac{p}{pref}}}$

In[312]:= $\alpha[1000, 1\, bar]$

Out[312]= 1.83723×10^{-39}

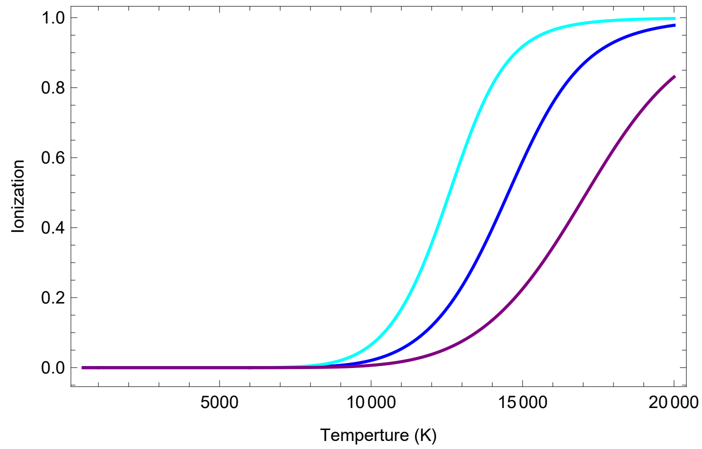
```
In[313]:= Alpha1bar = Plot[α[T, 1 bar], {T, 500, 20000}, PlotStyle → {Blue},
    PlotPoints → 200, Frame → True, FrameLabel → {"Temperture (K)", "Ionization"}];

In[314]:= Alpha0p1bar = Plot[α[T, 0.1 bar], {T, 500, 20000}, PlotStyle → {Cyan}, PlotPoints → 200,
    Frame → True, FrameLabel → {"Temperture (K)", "Ionization"}];

In[315]:= Alpha10bar = Plot[α[T, 10 bar], {T, 500, 20000}, PlotStyle → {Purple}, PlotPoints → 200,
    Frame → True, FrameLabel → {"Temperture (K)", "Ionization"}];
```

In[316]:=
```
Show[Alpha1bar, Alpha0p1bar, Alpha10bar]
```

Out[316]=



In[317]:=
```
TableForm[Table[{i * 1000, α[i * 1000, 0.1 bar] , α[i * 1000, 1 bar], α[i * 1000, 10 bar]},
  {i, 1, 20}], TableHeadings → {None, {"Temp (K)", "α 0.1 bar", "α 1 bar", "α 10 bar"}}]
```

Out[317]//TableForm=

Temp (K)	α 0.1 bar	α 1 bar	α 10 bar
1000	5.80982×10^{-39}	1.83723×10^{-39}	5.80982×10^{-40}
2000	1.04434×10^{-18}	3.3025×10^{-19}	1.04434×10^{-19}
3000	7.42577×10^{-12}	2.34823×10^{-12}	7.42577×10^{-13}
4000	2.20951×10^{-8}	6.98708×10^{-9}	2.20951×10^{-9}
5000	2.86022×10^{-6}	9.04481×10^{-7}	2.86022×10^{-7}
6000	0.0000763702	0.0000241504	7.63702×10^{-6}
7000	0.000822184	0.000259997	0.0000822184
8000	0.00499793	0.0015805	0.000499799
9000	0.0206991	0.0065469	0.00207035
10 000	0.0653096	0.0206925	0.00654479
11 000	0.167359	0.0536034	0.0169728
12 000	0.354538	0.119051	0.0378896
13 000	0.602213	0.232032	0.0752198
14 000	0.807549	0.397332	0.135654
15 000	0.917557	0.589486	0.224861
16 000	0.964635	0.756648	0.34367
17 000	0.983958	0.867524	0.482956
18 000	0.992204	0.929375	0.622864
19 000	0.995949	0.961579	0.74225
20 000	0.997763	0.978286	0.830783

Knowing alpha (degree of ionization), find mole fractions

In[318]:=
```
nTot[T_, P_] := (1 - α[T, P]) + 2 α[T, P]
```

In[319]:=
```
yAr[T_, P_] := (1 - α[T, P]) / nTot[T, P]
```

In[320]:=
```
yArII[T_, P_] := α[T, P] / nTot[T, P]
```

$$\mathtt{yArII[T\_,\ P\_]} := \frac{\alpha[T,\ P]}{\mathtt{nTot}[T,\ P]}$$

In[321]:=

$$\mathtt{ye[T\_,\ P\_]} := \frac{\alpha[T,\ P]}{\mathtt{nTot}[T,\ P]}$$

In[322]:=
```
TableForm[Table[{i * 1000, yAr[1000 * i, 0.1 bar] ,
   yArII[1000 * i, 0.1 bar], ye[1000 * i, 0.1 bar] }, {i, 1, 20}],
 TableHeadings → {None, {"Temp (K)", "yAr 0.1 bar", "yArII 0.1 bar", "ye 0.1 bar"}}]
```

Out[322]//TableForm=

Temp (K)	y_{Ar} 0.1 bar	y_{ArII} 0.1 bar	y_e 0.1 bar
1000	1.	5.80982×10^{-39}	5.80982×10^{-39}
2000	1.	1.04434×10^{-18}	1.04434×10^{-18}
3000	1.	7.42577×10^{-12}	7.42577×10^{-12}
4000	1.	2.20951×10^{-8}	2.20951×10^{-8}
5000	0.999994	2.86021×10^{-6}	2.86021×10^{-6}
6000	0.999847	0.0000763644	0.0000763644
7000	0.998357	0.000821508	0.000821508
8000	0.990054	0.00497308	0.00497308
9000	0.959441	0.0202794	0.0202794
10 000	0.877389	0.0613057	0.0613057
11 000	0.713269	0.143365	0.143365
12 000	0.476518	0.261741	0.261741
13 000	0.248274	0.375863	0.375863
14 000	0.10647	0.446765	0.446765
15 000	0.0429938	0.478503	0.478503
16 000	0.0180009	0.491	0.491
17 000	0.00808593	0.495957	0.495957
18 000	0.00391317	0.498043	0.498043
19 000	0.00202948	0.498985	0.498985
20 000	0.00111962	0.49944	0.49944

In[323]:=
```
TableForm[Table[
  {i * 1000, yAr[1000 * i, 1 bar] , yArII[1000 * i,  1 bar], ye[1000 * i,  1 bar] }, {i, 1, 20}],
 TableHeadings → {None, {"Temp (K)", "y_Ar 1 bar", "y_ArII 1 bar", "y_e 1 bar"}}]
```

Out[323]//TableForm=

Temp (K)	y_{Ar} 1 bar	y_{ArII} 1 bar	y_e 1 bar
1000	1.	1.83723×10^{-39}	1.83723×10^{-39}
2000	1.	3.3025×10^{-19}	3.3025×10^{-19}
3000	1.	2.34823×10^{-12}	2.34823×10^{-12}
4000	1.	6.98708×10^{-9}	6.98708×10^{-9}
5000	0.999998	9.0448×10^{-7}	9.0448×10^{-7}
6000	0.999952	0.0000241498	0.0000241498
7000	0.99948	0.00025993	0.00025993
8000	0.996844	0.00157801	0.00157801
9000	0.986991	0.00650432	0.00650432
10 000	0.959454	0.020273	0.020273
11 000	0.898247	0.0508763	0.0508763
12 000	0.787229	0.106385	0.106385
13 000	0.623335	0.188332	0.188332
14 000	0.431299	0.28435	0.28435
15 000	0.258268	0.370866	0.370866
16 000	0.138532	0.430734	0.430734
17 000	0.0709369	0.464532	0.464532
18 000	0.0366052	0.481697	0.481697
19 000	0.019587	0.490207	0.490207
20 000	0.0109764	0.494512	0.494512

In[324]:=
```
TableForm[Table[{i * 1000, yAr[1000 * i, 10 bar] ,
   yArII[1000 * i,  10 bar], ye[1000 * i,  10 bar] }, {i, 1, 20}],
 TableHeadings → {None, {"Temp  (K)", "y_Ar 10 bar", "y_ArII 10 bar", "y_e 10 bar"}}]
```

Out[324]//TableForm=

Temp (K)	y_{Ar} 10 bar	y_{ArII} 10 bar	y_e 10 bar
1000	1.	5.80982×10^{-40}	5.80982×10^{-40}
2000	1.	1.04434×10^{-19}	1.04434×10^{-19}
3000	1.	7.42577×10^{-13}	7.42577×10^{-13}
4000	1.	2.20951×10^{-9}	2.20951×10^{-9}
5000	0.999999	2.86022×10^{-7}	2.86022×10^{-7}
6000	0.999985	7.63696×10^{-6}	7.63696×10^{-6}
7000	0.999836	0.0000822116	0.0000822116
8000	0.999001	0.00049955	0.00049955
9000	0.995868	0.00206608	0.00206608
10 000	0.986996	0.00650224	0.00650224
11 000	0.966621	0.0166896	0.0166896
12 000	0.926987	0.0365064	0.0365064
13 000	0.860085	0.0699576	0.0699576
14 000	0.7611	0.11945	0.11945
15 000	0.632838	0.183581	0.183581
16 000	0.488461	0.25577	0.25577
17 000	0.348658	0.325671	0.325671
18 000	0.232389	0.383805	0.383805
19 000	0.147941	0.426029	0.426029
20 000	0.0924287	0.453786	0.453786

Check: These values are matching CEA exactly.

Average molecular weight of mixture (mole-weighted average of molecular weight of each species)

In[325]:=
```
MWavg[T_, P_] := yAr[T, P] MWar + yArII[T, P] MWarII + ye[T, P] MWe
```

Mixture enthalpy on mole basis (J/kmol)

In[326]:=
```
hmix[T_, P_] := yAr[T, P] h_Ar[T] +  yArII[T, P] h_ArII[T]  +  ye[T, P] h_e[T]
```

Mixture enthalpy on mass basis (J/kg)

In[327]:=
```
hmass[T_, P_] := hmix[T, P] / MWavg[T, P]
```

Equilibrium heat capacity (J/kg-K)

In[328]:=
```
cpmass[Tinput_, P_] := D[hmass[T, P], T] /. T → Tinput
```

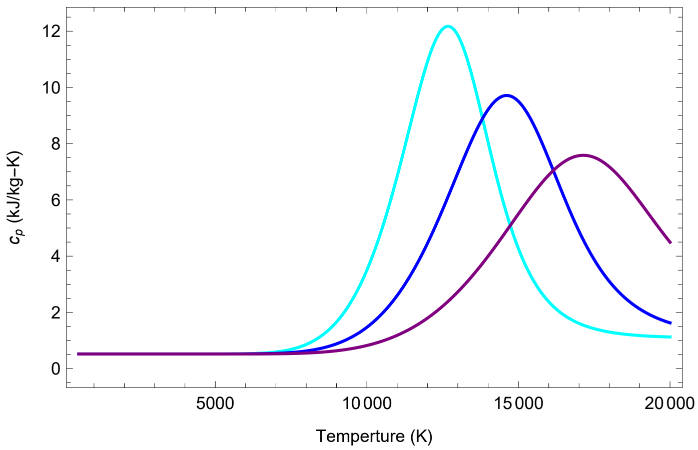
In[329]:=
```
Cp1bar  = Plot[Evaluate[cpmass[T, 1 bar] / kJ], {T, 500, 20000}, PlotStyle → {Blue},
   PlotPoints → 200, Frame → True, FrameLabel → {"Temperture  (K)", "c_p  (kJ/kg-K)"}];
```

In[330]:=
```
Cp0p1bar = Plot[Evaluate[cpmass[T, 0.1 bar] / kJ],
    {T, 500, 20000}, PlotStyle → {Cyan}, PlotPoints → 200,
    Frame → True, FrameLabel → {"Temperture (K)", "cp (kJ/kg-K)"}];
```

In[331]:=
```
Cp10bar = Plot[Evaluate[cpmass[T, 10 bar] / kJ],
    {T, 500, 20000}, PlotStyle → {Purple}, PlotPoints → 200,
    Frame → True, FrameLabel → {"Temperture (K)", "cp (kJ/kg-K)"}];
```

In[332]:=
```
Show[Cp0p1bar, Cp1bar, Cp10bar]
```

Out[332]=



In[333]:=
```
TableForm[Table[{i * 1000, cpmass[i * 1000, 0.1 bar] / kJ , cpmass[i * 1000, 1 bar] / kJ,
    cpmass[i * 1000, 10 bar] / kJ}, {i, 1, 20}], TableHeadings → {None,
    {"Temp (K)", "cp (kJ/kg-K) 0.1 bar", "cp (kJ/kg-K) 1 bar", "cp (kJ/kg-K) 10 bar"}}]
```

Out[333]//TableForm=

Temp (K)	c_p (kJ/kg-K) 0.1 bar	c_p (kJ/kg-K) 1 bar	c_p (kJ/kg-K) 10 bar
1000	0.520331	0.520331	0.520331
2000	0.520331	0.520331	0.520331
3000	0.520331	0.520331	0.520331
4000	0.520336	0.520333	0.520331
5000	0.520789	0.520476	0.520377
6000	0.529063	0.523092	0.521204
7000	0.591255	0.542753	0.527415
8000	0.858764	0.626961	0.553655
9000	1.65968	0.881431	0.635125
10 000	3.49799	1.46915	0.822341
11 000	6.83827	2.599	1.18374
12 000	10.9167	4.45604	1.79663
13 000	11.8561	6.95944	2.72896
14 000	8.05156	9.2153	4.00075
15 000	4.26496	9.50383	5.50284
16 000	2.37744	7.45018	6.88452
17 000	1.60756	4.88216	7.5734
18 000	1.30038	3.09867	7.17477
19 000	1.17541	2.12048	5.93292
20 000	1.12575	1.62708	4.49625

Check: These values are matching CEA exactly.

Equilibrium enthalpy (J/kg)

In[334]:=
```
h1bar = Plot[Evaluate[hmass[T, 1 bar] / MJ], {T, 500, 20000}, PlotStyle → {Blue},
    PlotPoints → 200, Frame → True, FrameLabel → {"Temperture (K)", "h (MJ/kg)"}];
```

In[335]:=
```
hp1bar = Plot[Evaluate[hmass[T, 0.1 bar] / MJ], {T, 500, 20000}, PlotStyle → {Cyan},
    PlotPoints → 200, Frame → True, FrameLabel → {"Temperture (K)", "h (MJ/kg)"}];
```

In[336]:=
```
h10bar = Plot[Evaluate[hmass[T, 10 bar] / MJ], {T, 500, 20000}, PlotStyle → {Purple},
    PlotPoints → 200, Frame → True, FrameLabel → {"Temperture (K)", "h (MJ/kg)"}];
```

In[337]:=
```
Show[hp1bar, h1bar, h10bar]
```

Out[337]=