29566428_FIT5149_Ass1

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1 FIT5149 Assessment 1

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2 Importing necessary Libraries

[1]:
```
library(psych) # for describe
library(lattice) # for levelplot
library(leaps) # for Regsubplots
require(ggplot2) # for various plots
```

```
Loading required package: ggplot2
Registered S3 methods overwritten by 'ggplot2':
  method         from
  [.quosures     rlang
  c.quosures     rlang
  print.quosures rlang

Attaching package: 'ggplot2'

The following objects are masked from 'package:psych':

    %+%, alpha
```

3 Loading Data

[2]:
```
data <- read.csv('train.csv', header = TRUE, sep = ',')
unique_m <- read.csv('unique_m.csv', header = TRUE, sep = ',')
```

Analysing the general Overview of the data

[3]:
```
head(data)
```

number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atomic_mass	wtd_gmean
4	88.94447	57.86269	66.36159	36.11661
5	92.72921	58.51842	73.13279	36.39660
4	88.94447	57.88524	66.36159	36.12251
4	88.94447	57.87397	66.36159	36.11956
4	88.94447	57.84014	66.36159	36.11072
4	88.94447	57.79504	66.36159	36.09893

[4]:
```
head(unique_m)
```

H	He	Li	Be	B	C	N	O	F	Ne	...	Au	Hg	Tl	Pb	Bi	Po	At	Rn	critical_temp	m
0	0	0	0	0	0	0	4	0	0	...	0	0	0	0	0	0	0	0	29	Ba
0	0	0	0	0	0	0	4	0	0	...	0	0	0	0	0	0	0	0	26	Ba
0	0	0	0	0	0	0	4	0	0	...	0	0	0	0	0	0	0	0	19	Ba
0	0	0	0	0	0	0	4	0	0	...	0	0	0	0	0	0	0	0	22	Ba
0	0	0	0	0	0	0	4	0	0	...	0	0	0	0	0	0	0	0	23	Ba
0	0	0	0	0	0	0	4	0	0	...	0	0	0	0	0	0	0	0	23	Ba

[5]:
```
print(paste("So there is about", dim(data)[1],"rows and␣
 ↪about",dim(data)[2],"columns in the Train data"))
```

```
[1] "So there is about 21263 rows and about 82 columns in the Train data"
```

[6]:
```
print(paste("So there is about", dim(unique_m)[1],"rows and␣
 ↪about",dim(unique_m)[2],"columns in the unique_m data"))
```

```
[1] "So there is about 21263 rows and about 88 columns in the unique_m data"
```

[7]:
```
round(describe(data),3)
```

	vars	n	mean	sd	median	trimmed	mad	min
number_of_elements	1	21263	4.115	1.439	4.000	4.106	1.483	1.00
mean_atomic_mass	2	21263	87.558	29.676	84.923	85.819	19.982	6.94
wtd_mean_atomic_mass	3	21263	72.988	33.490	60.697	68.406	18.414	6.42
gmean_atomic_mass	4	21263	71.291	31.030	66.362	67.623	15.261	5.32
wtd_gmean_atomic_mass	5	21263	58.540	36.651	39.918	52.085	15.273	1.96
entropy_atomic_mass	6	21263	1.166	0.365	1.200	1.192	0.361	0.00
wtd_entropy_atomic_mass	7	21263	1.064	0.401	1.147	1.093	0.375	0.00
range_atomic_mass	8	21263	115.601	54.627	122.906	118.755	60.825	0.00
wtd_range_atomic_mass	9	21263	33.225	26.968	26.636	28.696	16.090	0.00
std_atomic_mass	10	21263	44.392	20.035	45.123	45.335	19.200	0.00
wtd_std_atomic_mass	11	21263	41.448	19.984	44.286	42.074	17.239	0.00
mean_fie	12	21263	769.615	87.489	764.900	763.041	53.645	375
wtd_mean_fie	13	21263	870.442	143.278	889.967	879.073	174.453	375
gmean_fie	14	21263	737.475	78.327	727.961	730.173	53.584	375
wtd_gmean_fie	15	21263	832.770	119.773	856.203	839.543	128.169	375
entropy_fie	16	21263	1.299	0.382	1.356	1.325	0.384	0.00
wtd_entropy_fie	17	21263	0.927	0.334	0.917	0.924	0.223	0.00
range_fie	18	21263	572.223	309.614	764.100	592.974	68.941	0.00
wtd_range_fie	19	21263	483.517	224.043	510.440	494.860	278.398	0.00
std_fie	20	21263	215.631	109.967	266.374	221.657	78.452	0.00
wtd_std_fie	21	21263	224.050	127.927	258.450	233.091	136.543	0.00
mean_atomic_radius	22	21263	157.983	20.147	160.250	159.018	15.493	48.0
wtd_mean_atomic_radius	23	21263	134.720	28.802	125.970	132.333	28.835	48.0
gmean_atomic_radius	24	21263	144.449	22.091	142.808	144.246	15.886	48.0
wtd_gmean_atomic_radius	25	21263	120.989	35.838	113.181	117.557	39.648	48.0
entropy_atomic_radius	26	21263	1.268	0.375	1.331	1.292	0.351	0.00
wtd_entropy_atomic_radius	27	21263	1.131	0.407	1.243	1.167	0.351	0.00
range_atomic_radius	28	21263	139.325	67.272	171.000	146.801	50.408	0.00
wtd_range_atomic_radius	29	21263	51.370	35.019	43.000	45.729	22.650	0.00
std_atomic_radius	30	21263	51.601	22.898	58.663	53.766	18.736	0.00
...	...	...	...	...	...	...	...	...
wtd_mean_FusionHeat	53	21263	13.848	14.279	8.331	10.956	5.684	0.22
gmean_FusionHeat	54	21263	10.137	10.066	5.253	8.161	2.630	0.22
wtd_gmean_FusionHeat	55	21263	10.141	13.134	4.930	7.631	5.489	0.22
entropy_FusionHeat	56	21263	1.093	0.376	1.112	1.114	0.395	0.00
wtd_entropy_FusionHeat	57	21263	0.914	0.370	0.995	0.938	0.334	0.00
range_FusionHeat	58	21263	21.139	20.371	12.878	16.902	5.281	0.00
wtd_range_FusionHeat	59	21263	8.219	11.414	3.436	5.913	2.626	0.00
std_FusionHeat	60	21263	8.323	8.672	4.948	6.386	1.675	0.00
wtd_std_FusionHeat	61	21263	7.718	7.288	5.501	6.232	1.839	0.00
mean_ThermalConductivity	62	21263	89.707	38.517	96.504	89.978	29.594	0.02
wtd_mean_ThermalConductivity	63	21263	81.549	45.519	73.333	76.951	35.972	0.02
gmean_ThermalConductivity	64	21263	29.842	34.060	14.288	23.034	10.815	0.02
wtd_gmean_ThermalConductivity	65	21263	27.308	40.191	6.096	19.120	8.119	0.02
entropy_ThermalConductivity	66	21263	0.728	0.326	0.739	0.731	0.376	0.00
wtd_entropy_ThermalConductivity	67	21263	0.540	0.318	0.546	0.524	0.398	0.00
range_ThermalConductivity	68	21263	250.893	158.704	399.795	261.322	4.144	0.00
wtd_range_ThermalConductivity	69	21263	62.033	43.123	56.556	57.775	45.729	0.00
std_ThermalConductivity	70	21263	98.944	60.143	135.762	101.303	50.056	0.00
wtd_std_ThermalConductivity	71	21263	96.234	63.710	113.557	97.354	80.255	0.00
mean_Valence	72	21263	3.198	1.045	2.833	3.061	0.865	1.00
wtd_mean_Valence	73	21263	3.153	1.191	2.618	2.993	0.802	1.00

[8]:
```
round(describe(unique_m),3)
```

	vars	n	mean	sd	median	trimmed	mad	min	max	range
H	1	21263	0.018	0.267	0.0	0.000	0.000	0	14.000	14.00
He	2	21263	0.000	0.000	0.0	0.000	0.000	0	0.000	0.000
Li	3	21263	0.012	0.130	0.0	0.000	0.000	0	3.000	3.000
Be	4	21263	0.035	0.849	0.0	0.000	0.000	0	40.000	40.00
B	5	21263	0.143	1.044	0.0	0.000	0.000	0	105.000	105.0
C	6	21263	0.385	4.408	0.0	0.000	0.000	0	120.000	120.0
N	7	21263	0.013	0.150	0.0	0.000	0.000	0	12.800	12.80
O	8	21263	3.009	3.812	1.0	2.528	1.483	0	66.000	66.00
F	9	21263	0.015	0.132	0.0	0.000	0.000	0	4.000	4.000
Ne	10	21263	0.000	0.000	0.0	0.000	0.000	0	0.000	0.000
Na	11	21263	0.009	0.102	0.0	0.000	0.000	0	4.000	4.000
Mg	12	21263	0.027	0.272	0.0	0.000	0.000	0	12.000	12.00
Al	13	21263	0.062	1.126	0.0	0.000	0.000	0	99.925	99.92
Si	14	21263	0.190	2.217	0.0	0.000	0.000	0	100.000	100.0
P	15	21263	0.028	0.467	0.0	0.000	0.000	0	20.000	20.00
S	16	21263	0.106	0.761	0.0	0.000	0.000	0	15.000	15.00
Cl	17	21263	0.009	0.120	0.0	0.000	0.000	0	3.000	3.000
Ar	18	21263	0.000	0.000	0.0	0.000	0.000	0	0.000	0.000
K	19	21263	0.016	0.138	0.0	0.000	0.000	0	3.300	3.300
Ca	20	21263	0.258	0.903	0.0	0.054	0.000	0	24.000	24.00
Sc	21	21263	0.011	0.186	0.0	0.000	0.000	0	5.000	5.000
Ti	22	21263	0.157	2.728	0.0	0.000	0.000	0	75.000	75.00
V	23	21263	0.225	3.408	0.0	0.000	0.000	0	79.500	79.50
Cr	24	21263	0.006	0.254	0.0	0.000	0.000	0	34.900	34.90
Mn	25	21263	0.003	0.129	0.0	0.000	0.000	0	14.000	14.00
Fe	26	21263	0.153	0.713	0.0	0.000	0.000	0	30.000	30.00
Co	27	21263	0.035	0.581	0.0	0.000	0.000	0	35.380	35.38
Ni	28	21263	0.090	0.983	0.0	0.000	0.000	0	45.000	45.00
Cu	29	21263	1.277	2.079	0.9	1.053	1.334	0	98.000	98.00
Zn	30	21263	0.014	0.403	0.0	0.000	0.000	0	20.000	20.00
...	...	...	...	...	...	...	...	...	...	...
Pr	59	21263	0.041	1.282	0	0.000	0.000	0	185.00	185.0
Nd	60	21263	0.040	0.225	0	0.000	0.000	0	6.00	6.00
Pm	61	21263	0.000	0.000	0	0.000	0.000	0	0.00	0.00
Sm	62	21263	0.022	0.183	0	0.000	0.000	0	12.00	12.00
Eu	63	21263	0.018	0.151	0	0.000	0.000	0	6.00	6.00
Gd	64	21263	0.024	0.156	0	0.000	0.000	0	4.00	4.00
Tb	65	21263	0.003	0.065	0	0.000	0.000	0	5.00	5.00
Dy	66	21263	0.010	0.104	0	0.000	0.000	0	5.00	5.00
Ho	67	21263	0.009	0.099	0	0.000	0.000	0	5.00	5.00
Er	68	21263	0.014	0.131	0	0.000	0.000	0	5.00	5.00
Tm	69	21263	0.009	0.130	0	0.000	0.000	0	5.00	5.00
Yb	70	21263	0.013	0.215	0	0.000	0.000	0	16.00	16.00
Lu	71	21263	0.027	0.277	0	0.000	0.000	0	7.00	7.00
Hf	72	21263	0.009	0.209	0	0.000	0.000	0	25.00	25.00
Ta	73	21263	0.036	0.851	0	0.000	0.000	0	55.00	55.00
W	74	21263	0.010	0.165	0	0.000	0.000	0	14.00	14.00
Re	75	21263	0.038	1.177	0	0.000	0.000	0	97.24	97.24
Os	76	21263	0.023	0.282	0	0.000	0.000	0	10.00	10.00
Ir	77	21263	0.062	0.865	0	0.000	0.000	0	45.00	45.00
Pt	78	21263	0.034	0.308	0	0.000	0.000	0	5.80	5.80
Au	79	21263	0.021	0.718	0	0.000	0.000	0	64.00	64.00

[9]:
```
str(data)
```

```
'data.frame':   21263 obs. of  82 variables:
 $ number_of_elements            : int  4 5 4 4 4 4 4 4 4 4 ...
 $ mean_atomic_mass              : num  88.9 92.7 88.9 88.9 88.9 ...
 $ wtd_mean_atomic_mass          : num  57.9 58.5 57.9 57.9 57.8 ...
 $ gmean_atomic_mass             : num  66.4 73.1 66.4 66.4 66.4 ...
 $ wtd_gmean_atomic_mass         : num  36.1 36.4 36.1 36.1 36.1 ...
 $ entropy_atomic_mass           : num  1.18 1.45 1.18 1.18 1.18 ...
 $ wtd_entropy_atomic_mass       : num  1.062 1.058 0.976 1.022 1.129 ...
 $ range_atomic_mass             : num  123 123 123 123 123 ...
 $ wtd_range_atomic_mass         : num  31.8 36.2 35.7 33.8 27.8 ...
 $ std_atomic_mass               : num  52 47.1 52 52 52 ...
 $ wtd_std_atomic_mass           : num  53.6 54 53.7 53.6 53.6 ...
 $ mean_fie                      : num  775 766 775 775 775 ...
 $ wtd_mean_fie                  : num  1010 1011 1011 1011 1010 ...
 $ gmean_fie                     : num  718 721 718 718 718 ...
 $ wtd_gmean_fie                 : num  938 939 939 939 937 ...
 $ entropy_fie                   : num  1.31 1.54 1.31 1.31 1.31 ...
 $ wtd_entropy_fie               : num  0.791 0.807 0.774 0.783 0.805 ...
 $ range_fie                     : num  811 811 811 811 811 ...
 $ wtd_range_fie                 : num  736 743 743 740 729 ...
 $ std_fie                       : num  324 290 324 324 324 ...
 $ wtd_std_fie                   : num  356 355 355 355 356 ...
 $ mean_atomic_radius            : num  160 161 160 160 160 ...
 $ wtd_mean_atomic_radius        : num  106 105 105 105 106 ...
 $ gmean_atomic_radius           : num  136 141 136 136 136 ...
 $ wtd_gmean_atomic_radius       : num  84.5 84.4 84.2 84.4 84.8 ...
 $ entropy_atomic_radius         : num  1.26 1.51 1.26 1.26 1.26 ...
 $ wtd_entropy_atomic_radius     : num  1.21 1.2 1.13 1.17 1.26 ...
 $ range_atomic_radius           : int  205 205 205 205 205 205 205 171 171 171
...
 $ wtd_range_atomic_radius       : num  42.9 50.6 49.3 46.1 36.5 ...
 $ std_atomic_radius             : num  75.2 67.3 75.2 75.2 75.2 ...
 $ wtd_std_atomic_radius         : num  69.2 68 67.8 68.5 70.6 ...
 $ mean_Density                  : num  4654 5821 4654 4654 4654 ...
 $ wtd_mean_Density              : num  2962 3021 2999 2980 2924 ...
 $ gmean_Density                 : num  725 1237 725 725 725 ...
 $ wtd_gmean_Density             : num  53.5 54.1 54 53.8 53.1 ...
 $ entropy_Density               : num  1.03 1.31 1.03 1.03 1.03 ...
 $ wtd_entropy_Density           : num  0.815 0.915 0.76 0.789 0.86 ...
 $ range_Density                 : num  8959 10489 8959 8959 8959 ...
 $ wtd_range_Density             : num  1580 1667 1667 1623 1492 ...
 $ std_Density                   : num  3306 3767 3306 3306 3306 ...
 $ wtd_std_Density               : num  3573 3633 3592 3582 3553 ...
 $ mean_ElectronAffinity         : num  81.8 90.9 81.8 81.8 81.8 ...
 $ wtd_mean_ElectronAffinity     : num  112 112 112 112 111 ...
```

```
 $ gmean_ElectronAffinity         : num  60.1 69.8 60.1 60.1 60.1 ...
 $ wtd_gmean_ElectronAffinity     : num  99.4 101.2 101.1 100.2 97.8 ...
 $ entropy_ElectronAffinity       : num  1.16 1.43 1.16 1.16 1.16 ...
 $ wtd_entropy_ElectronAffinity   : num  0.787 0.839 0.786 0.787 0.787 ...
 $ range_ElectronAffinity         : num  127 127 127 127 127 ...
 $ wtd_range_ElectronAffinity     : num  81 81.2 81.2 81.1 80.8 ...
 $ std_ElectronAffinity           : num  51.4 49.4 51.4 51.4 51.4 ...
 $ wtd_std_ElectronAffinity       : num  42.6 41.7 41.6 42.1 43.5 ...
 $ mean_FusionHeat                : num  6.91 7.78 6.91 6.91 6.91 ...
 $ wtd_mean_FusionHeat            : num  3.85 3.8 3.82 3.83 3.87 ...
 $ gmean_FusionHeat               : num  3.48 4.4 3.48 3.48 3.48 ...
 $ wtd_gmean_FusionHeat           : num  1.04 1.04 1.04 1.04 1.04 ...
 $ entropy_FusionHeat             : num  1.09 1.37 1.09 1.09 1.09 ...
 $ wtd_entropy_FusionHeat         : num  0.995 1.073 0.927 0.964 1.045 ...
 $ range_FusionHeat               : num  12.9 12.9 12.9 12.9 12.9 ...
 $ wtd_range_FusionHeat           : num  1.74 1.6 1.76 1.74 1.74 ...
 $ std_FusionHeat                 : num  4.6 4.47 4.6 4.6 4.6 ...
 $ wtd_std_FusionHeat             : num  4.67 4.6 4.65 4.66 4.68 ...
 $ mean_ThermalConductivity       : num  108 172 108 108 108 ...
 $ wtd_mean_ThermalConductivity   : num  61 61.4 60.9 61 61.1 ...
 $ gmean_ThermalConductivity      : num  7.06 16.06 7.06 7.06 7.06 ...
 $ wtd_gmean_ThermalConductivity  : num  0.622 0.62 0.619 0.621 0.625 ...
 $ entropy_ThermalConductivity    : num  0.308 0.847 0.308 0.308 0.308 ...
 $ wtd_entropy_ThermalConductivity: num  0.263 0.568 0.25 0.257 0.273 ...
 $ range_ThermalConductivity      : num  400 430 400 400 400 ...
 $ wtd_range_ThermalConductivity  : num  57.1 51.4 57.1 57.1 57.1 ...
 $ std_ThermalConductivity        : num  169 199 169 169 169 ...
 $ wtd_std_ThermalConductivity    : num  139 140 139 139 138 ...
 $ mean_Valence                   : num  2.25 2 2.25 2.25 2.25 2.25 2.25 2.25
2.25 2.25 ...
 $ wtd_mean_Valence               : num  2.26 2.26 2.27 2.26 2.24 ...
 $ gmean_Valence                  : num  2.21 1.89 2.21 2.21 2.21 ...
 $ wtd_gmean_Valence              : num  2.22 2.21 2.23 2.23 2.21 ...
 $ entropy_Valence                : num  1.37 1.56 1.37 1.37 1.37 ...
 $ wtd_entropy_Valence            : num  1.07 1.05 1.03 1.05 1.1 ...
 $ range_Valence                  : int  1 2 1 1 1 1 1 1 1 1 ...
 $ wtd_range_Valence              : num  1.09 1.13 1.11 1.1 1.06 ...
 $ std_Valence                    : num  0.433 0.632 0.433 0.433 0.433 ...
 $ wtd_std_Valence                : num  0.437 0.469 0.445 0.441 0.429 ...
 $ critical_temp                  : num  29 26 19 22 23 23 11 33 36 31 ...
```

We can See that all the variables are numeric or continous Variable

[10]:
```
str(unique_m)
```

```
'data.frame':   21263 obs. of  88 variables:
 $ H            : num  0 0 0 0 0 0 0 0 0 0 ...
 $ He           : int  0 0 0 0 0 0 0 0 0 0 ...
 $ Li           : num  0 0 0 0 0 0 0 0 0 0 ...
```

```
$ Be            : num  0 0 0 0 0 0 0 0 0 0 ...
$ B             : num  0 0 0 0 0 0 0 0 0 0 ...
$ C             : num  0 0 0 0 0 0 0 0 0 0 ...
$ N             : num  0 0 0 0 0 0 0 0 0 0 ...
$ O             : num  4 4 4 4 4 4 4 4 4 4 ...
$ F             : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ne            : int  0 0 0 0 0 0 0 0 0 0 ...
$ Na            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Mg            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Al            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Si            : num  0 0 0 0 0 0 0 0 0 0 ...
$ P             : num  0 0 0 0 0 0 0 0 0 0 ...
$ S             : num  0 0 0 0 0 0 0 0 0 0 ...
$ Cl            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ar            : int  0 0 0 0 0 0 0 0 0 0 ...
$ K             : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ca            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Sc            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ti            : num  0 0 0 0 0 0 0 0 0 0 ...
$ V             : num  0 0 0 0 0 0 0 0 0 0 ...
$ Cr            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Mn            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Fe            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Co            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ni            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Cu            : num  1 0.9 1 1 1 1 1 1 1 1 ...
$ Zn            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ga            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ge            : num  0 0 0 0 0 0 0 0 0 0 ...
$ As            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Se            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Br            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Kr            : int  0 0 0 0 0 0 0 0 0 0 ...
$ Rb            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Sr            : num  0 0 0 0 0 0 0 0.1 0.15 0.2 ...
$ Y             : num  0 0 0 0 0 0 0 0 0 0 ...
$ Zr            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Nb            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Mo            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Tc            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ru            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Rh            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Pd            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Ag            : num  0 0.1 0 0 0 0 0 0 0 0 ...
$ Cd            : num  0 0 0 0 0 0 0 0 0 0 ...
$ In            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Sn            : num  0 0 0 0 0 0 0 0 0 0 ...
$ Sb            : num  0 0 0 0 0 0 0 0 0 0 ...
```

```
 $ Te           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ I            : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Xe           : int  0 0 0 0 0 0 0 0 0 0 ...
 $ Cs           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Ba           : num  0.2 0.1 0.1 0.15 0.3 0.5 1 0 0 0 ...
 $ La           : num  1.8 1.9 1.9 1.85 1.7 1.5 1 1.9 1.85 1.8 ...
 $ Ce           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Pr           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Nd           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Pm           : int  0 0 0 0 0 0 0 0 0 0 ...
 $ Sm           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Eu           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Gd           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Tb           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Dy           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Ho           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Er           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Tm           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Yb           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Lu           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Hf           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Ta           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ W            : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Re           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Os           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Ir           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Pt           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Au           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Hg           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Tl           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Pb           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Bi           : num  0 0 0 0 0 0 0 0 0 0 ...
 $ Po           : int  0 0 0 0 0 0 0 0 0 0 ...
 $ At           : int  0 0 0 0 0 0 0 0 0 0 ...
 $ Rn           : int  0 0 0 0 0 0 0 0 0 0 ...
 $ critical_temp: num  29 26 19 22 23 23 11 33 36 31 ...
 $ material     : Factor w/ 15542 levels "Ag0.002Al0.998",..: 518 509 512 504
528 592 950 11890 11888 11901 ...
```

3.1 Analysing Correlation between predictors and critical_temp

Extracting just the list of predictors with correlation value greater than 0.5 or less than -0.5 with critical_Temp

[11]:
```
correlationValues = c()
correlationName = c()
correlationSign = c()
absoluteCorrelationValue = c()
```

```
for(var1 in names(data)){
    if(cor(data[var1],data['critical_temp'])>0.5 ||␣
 ↪cor(data[var1],data['critical_temp'])< -0.5 ){
        corVal <- cor(data[var1],data['critical_temp'])
        correlationValues <- c(correlationValues, corVal)
        correlationName <- c(correlationName,var1)
        if(corVal > 0){
            correlationSign <- c(correlationSign,"+ve Correlation")
        }
        else{
                correlationSign <- c(correlationSign,"-ve Correlation")
        }
        absoluteCorrelationValue <-␣
 ↪c(absoluteCorrelationValue,abs(cor(data[var1],data['critical_temp'])))
    }
}
temp = data.
 ↪frame(correlationName,correlationValues,absoluteCorrelationValue,correlationSign)
correlation = temp[order(-temp$absoluteCorrelationValue),]
correlation
```

	correlationName	correlationValues	absoluteCorrelationValue	correlationSign
26	critical_temp	1.0000000	1.0000000	+ve Correlation
19	wtd_std_ThermalConductivity	0.7212711	0.7212711	+ve Correlation
17	range_ThermalConductivity	0.6876539	0.6876539	+ve Correlation
10	range_atomic_radius	0.6537590	0.6537590	+ve Correlation
18	std_ThermalConductivity	0.6536320	0.6536320	+ve Correlation
21	wtd_mean_Valence	-0.6324010	0.6324010	-ve Correlation
3	wtd_entropy_atomic_mass	0.6269304	0.6269304	+ve Correlation
23	wtd_gmean_Valence	-0.6156533	0.6156533	-ve Correlation
9	wtd_entropy_atomic_radius	0.6034940	0.6034940	+ve Correlation
1	number_of_elements	0.6010686	0.6010686	+ve Correlation
5	range_fie	0.6007904	0.6007904	+ve Correlation
20	mean_Valence	-0.6000849	0.6000849	-ve Correlation
12	wtd_std_atomic_radius	0.5991987	0.5991987	+ve Correlation
24	entropy_Valence	0.5985909	0.5985909	+ve Correlation
25	wtd_entropy_Valence	0.5896637	0.5896637	+ve Correlation
7	wtd_std_fie	0.5820133	0.5820133	+ve Correlation
22	gmean_Valence	-0.5730681	0.5730681	-ve Correlation
4	entropy_fie	0.5678169	0.5678169	+ve Correlation
16	wtd_entropy_FusionHeat	0.5632443	0.5632443	+ve Correlation
11	std_atomic_radius	0.5596286	0.5596286	+ve Correlation
8	entropy_atomic_radius	0.5589374	0.5589374	+ve Correlation
15	entropy_FusionHeat	0.5527087	0.5527087	+ve Correlation
2	entropy_atomic_mass	0.5436194	0.5436194	+ve Correlation
6	std_fie	0.5418038	0.5418038	+ve Correlation
13	gmean_Density	-0.5416844	0.5416844	-ve Correlation
14	wtd_gmean_Density	-0.5400456	0.5400456	-ve Correlation

Extracting the correlation data excluding critical temp column

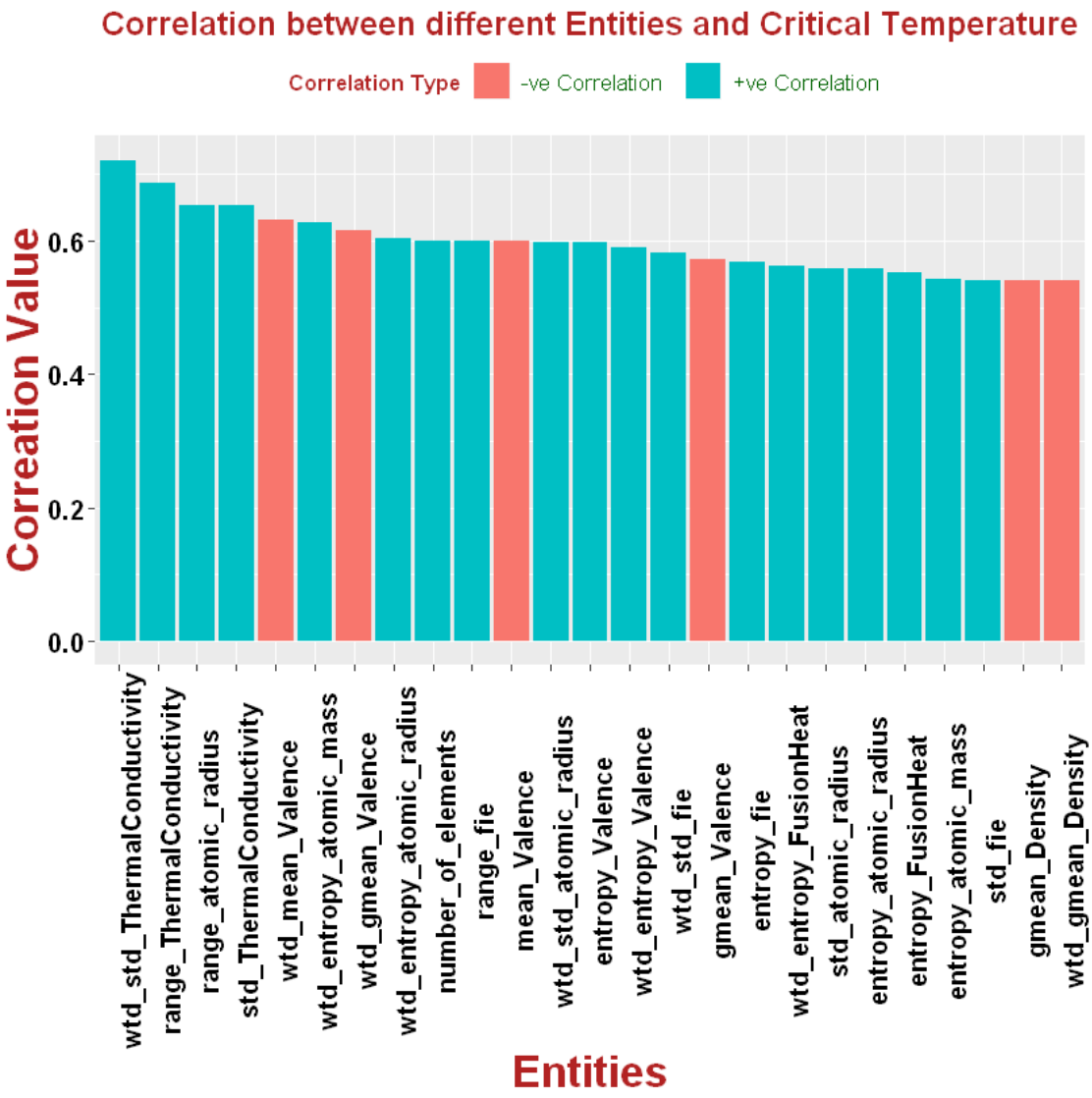
[12]:
```
correlationWithoutCriricalTemp = correlation[correlation$correlationName!
 ↪='critical_temp',]
correlationWithoutCriricalTemp
```

	correlationName	correlationValues	absoluteCorrelationValue	correlationSign
19	wtd_std_ThermalConductivity	0.7212711	0.7212711	+ve Correlation
17	range_ThermalConductivity	0.6876539	0.6876539	+ve Correlation
10	range_atomic_radius	0.6537590	0.6537590	+ve Correlation
18	std_ThermalConductivity	0.6536320	0.6536320	+ve Correlation
21	wtd_mean_Valence	-0.6324010	0.6324010	-ve Correlation
3	wtd_entropy_atomic_mass	0.6269304	0.6269304	+ve Correlation
23	wtd_gmean_Valence	-0.6156533	0.6156533	-ve Correlation
9	wtd_entropy_atomic_radius	0.6034940	0.6034940	+ve Correlation
1	number_of_elements	0.6010686	0.6010686	+ve Correlation
5	range_fie	0.6007904	0.6007904	+ve Correlation
20	mean_Valence	-0.6000849	0.6000849	-ve Correlation
12	wtd_std_atomic_radius	0.5991987	0.5991987	+ve Correlation
24	entropy_Valence	0.5985909	0.5985909	+ve Correlation
25	wtd_entropy_Valence	0.5896637	0.5896637	+ve Correlation
7	wtd_std_fie	0.5820133	0.5820133	+ve Correlation
22	gmean_Valence	-0.5730681	0.5730681	-ve Correlation
4	entropy_fie	0.5678169	0.5678169	+ve Correlation
16	wtd_entropy_FusionHeat	0.5632443	0.5632443	+ve Correlation
11	std_atomic_radius	0.5596286	0.5596286	+ve Correlation
8	entropy_atomic_radius	0.5589374	0.5589374	+ve Correlation
15	entropy_FusionHeat	0.5527087	0.5527087	+ve Correlation
2	entropy_atomic_mass	0.5436194	0.5436194	+ve Correlation
6	std_fie	0.5418038	0.5418038	+ve Correlation
13	gmean_Density	-0.5416844	0.5416844	-ve Correlation
14	wtd_gmean_Density	-0.5400456	0.5400456	-ve Correlation

[13]:
```
correlationWithoutCriricalTemp$correlationName <-␣
 ↪factor(correlationWithoutCriricalTemp$correlationName, levels =␣
 ↪correlationWithoutCriricalTemp$correlationName[order(-correlationWithoutCriricalTemp$absolu
```

[14]:
```
ggplot(data = correlationWithoutCriricalTemp , aes(x=␣
 ↪correlationWithoutCriricalTemp$correlationName, y=␣
 ↪correlationWithoutCriricalTemp$absoluteCorrelationValue))+
     theme_grey()+
     theme(axis.text = element_text(face="bold", color="Black",size=12,␣
 ↪angle=90),
           axis.text.y = element_text(angle = 0),
           axis.title = element_text(face="bold", color="firebrick",size=20),
           strip.text = element_text(size = 20, colour =␣
 ↪"DarkGreen",face="bold"),
           legend.title = element_text(size=10, color = "firebrick",face =␣
 ↪"bold"),
```

```
          legend.text = element_text(size=10,colour = "DarkGreen"),
          legend.position="top",
          plot.title =  element_text(size=15, color = "firebrick",face =␣
↪"bold",hjust = .5)) +
          labs(fill ="Correlation Type" ) +
          xlab("Entities") + ylab("Correation Value")+
          ggtitle("Correlation between different Entities and Critical␣
↪Temperature")+
          geom_col(aes(fill = correlationWithoutCriricalTemp$correlationSign)
      )
```



3.1.1 Extracting a new dataset from the original data set with only the highly correlated columns

[15]:
```
newData = data[,levels(correlation$correlationName)]
head(newData)
```

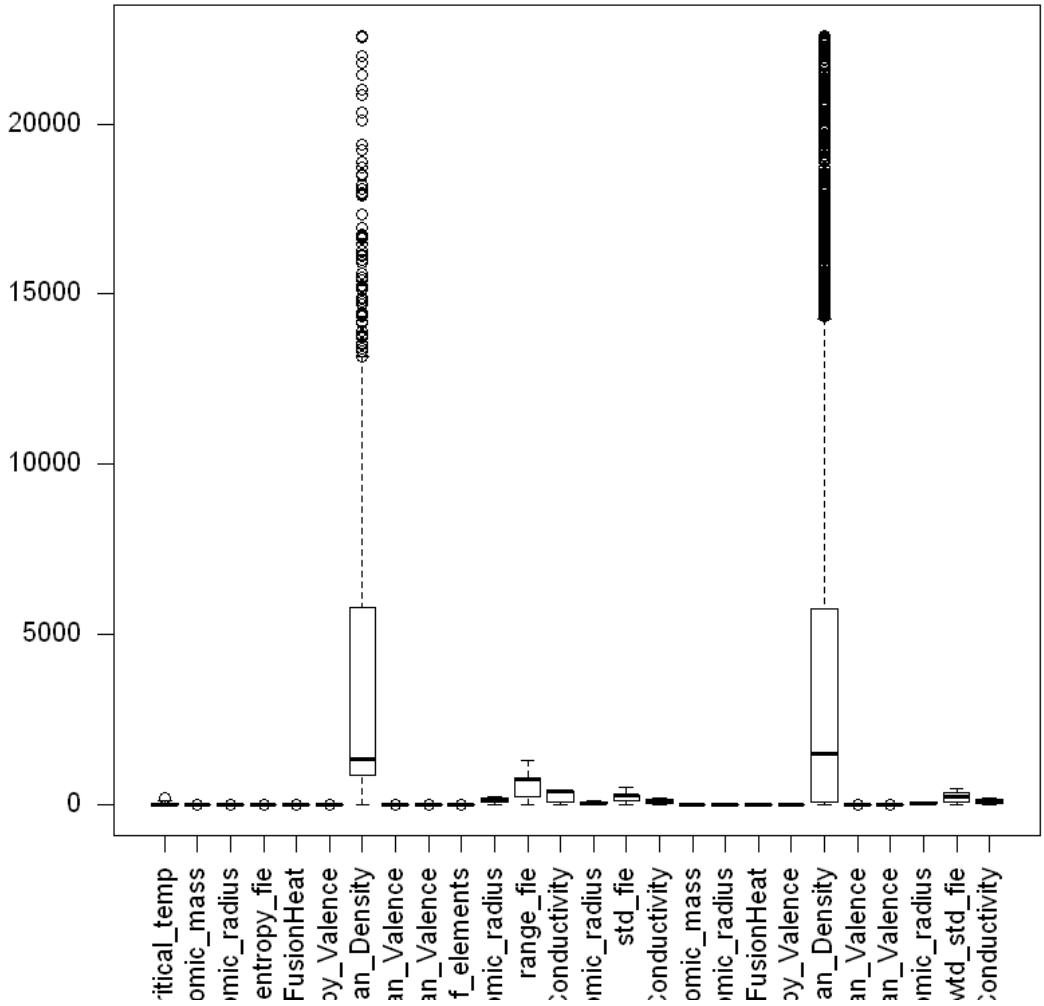
critical_temp	entropy_atomic_mass	entropy_atomic_radius	entropy_fie	entropy_FusionHeat	entro
29	1.181795	1.259244	1.305967	1.088575	1.368
26	1.449309	1.508328	1.544145	1.374977	1.557
19	1.181795	1.259244	1.305967	1.088575	1.368
22	1.181795	1.259244	1.305967	1.088575	1.368
23	1.181795	1.259244	1.305967	1.088575	1.368
23	1.181795	1.259244	1.305967	1.088575	1.368

Doing a basic analysis on the data

[16]:
```
round(describe(newData),3)
```

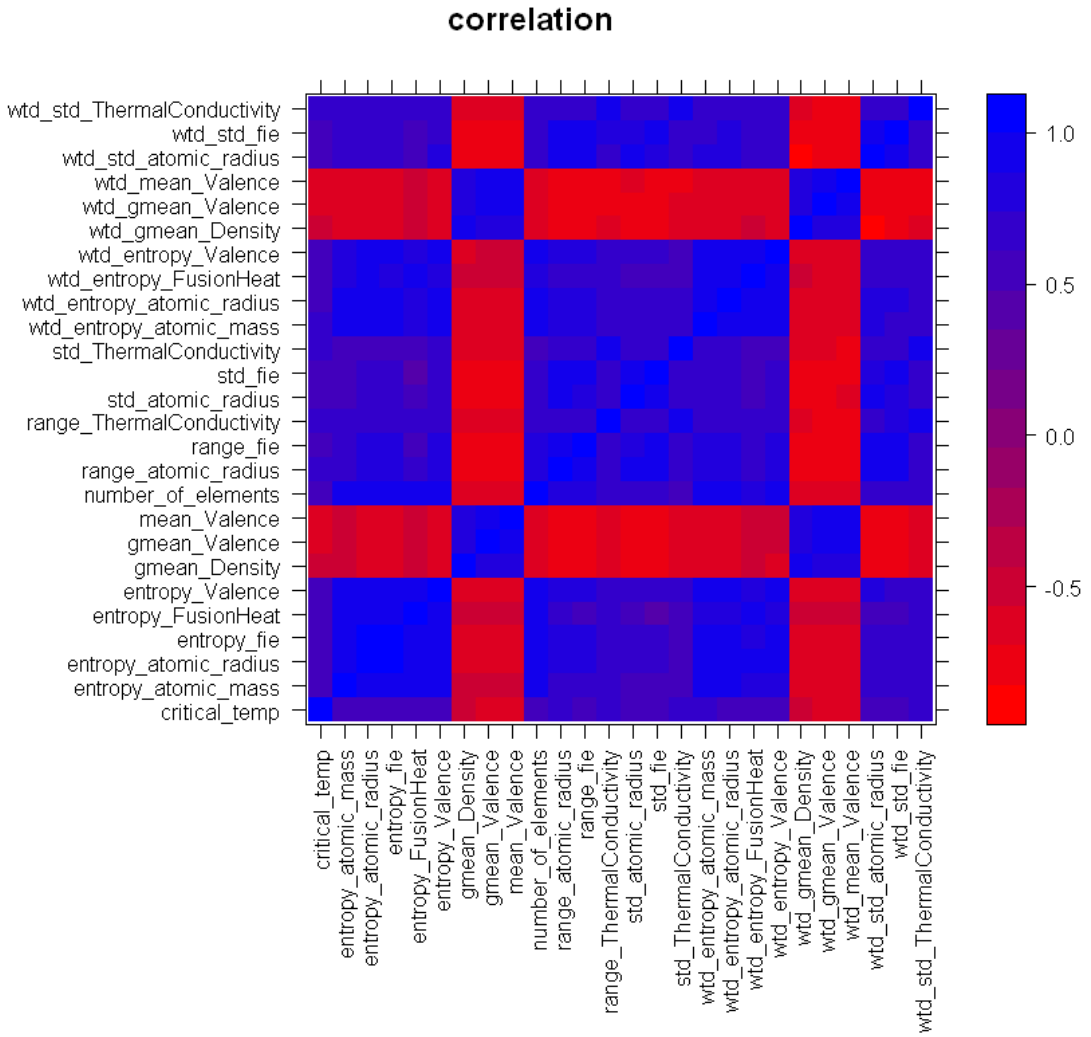
	vars	n	mean	sd	median	trimmed	mad	min
critical_temp	1	21263	34.421	34.254	20.000	30.314	25.412	0.00
entropy_atomic_mass	2	21263	1.166	0.365	1.200	1.192	0.361	0.00
entropy_atomic_radius	3	21263	1.268	0.375	1.331	1.292	0.351	0.00
entropy_fie	4	21263	1.299	0.382	1.356	1.325	0.384	0.00
entropy_FusionHeat	5	21263	1.093	0.376	1.112	1.114	0.395	0.00
entropy_Valence	6	21263	1.296	0.393	1.369	1.323	0.406	0.00
gmean_Density	7	21263	3460.692	3703.256	1339.975	2830.865	1078.960	1.42
gmean_Valence	8	21263	3.057	1.046	2.615	2.902	0.662	1.00
mean_Valence	9	21263	3.198	1.045	2.833	3.061	0.865	1.00
number_of_elements	10	21263	4.115	1.439	4.000	4.106	1.483	1.00
range_atomic_radius	11	21263	139.325	67.272	171.000	146.801	50.408	0.00
range_fie	12	21263	572.223	309.614	764.100	592.974	68.941	0.00
range_ThermalConductivity	13	21263	250.893	158.704	399.795	261.322	4.144	0.00
std_atomic_radius	14	21263	51.601	22.898	58.663	53.766	18.736	0.00
std_fie	15	21263	215.631	109.967	266.374	221.657	78.452	0.00
std_ThermalConductivity	16	21263	98.944	60.143	135.762	101.303	50.056	0.00
wtd_entropy_atomic_mass	17	21263	1.064	0.401	1.147	1.093	0.375	0.00
wtd_entropy_atomic_radius	18	21263	1.131	0.407	1.243	1.167	0.351	0.00
wtd_entropy_FusionHeat	19	21263	0.914	0.370	0.995	0.938	0.334	0.00
wtd_entropy_Valence	20	21263	1.053	0.380	1.167	1.084	0.319	0.00
wtd_gmean_Density	21	21263	3117.241	3975.123	1515.365	2430.880	2164.200	0.68
wtd_gmean_Valence	22	21263	3.056	1.175	2.434	2.881	0.560	1.00
wtd_mean_Valence	23	21263	3.153	1.191	2.618	2.993	0.802	1.00
wtd_std_atomic_radius	24	21263	52.340	25.295	59.933	54.726	26.004	0.00
wtd_std_fie	25	21263	224.050	127.927	258.450	233.091	136.543	0.00
wtd_std_ThermalConductivity	26	21263	96.234	63.710	113.557	97.354	80.255	0.00

[17]:
```
boxplot(newData, las=2, cex.axis = 1)
```



Now Lets check the correlation between all columns in the new dataset

[18]:
```
#Define the color scheme
cols = colorRampPalette(c("red","blue"))
#Plot the correlation matrix.
levelplot(cor(newData), col.regions = cols(100), main = "correlation", xlab =␣
↪NULL, ylab = NULL,
          scales = list(x = list(rot = 90)))
```



From this plot it looks like most of the columns are highly correlated to each other. So lets try to extract the values with correlation greater than 0.8 or less than 0.8

[19]:
```
used = c('critical_temp')
correlationValues = c()
correlationName = c()
correlationSign = c()
absoluteCorrelationValue = c()
for(entity in names(newData)){
    if(entity == 'critical_temp'){
        next
    }
    used = c(used,entity)
    for(var1 in names(newData)){
```

```
        if(is.element(var1, used)){
            next
        }
        if((var1!=entity) &&(cor(data[var1],data[entity])>0.8 ||␣
 ↪cor(data[var1],data[entity])< -0.8 )){
            corVal <- cor(data[var1],data[entity])
            correlationValues <- c(correlationValues, corVal)
            correlationName <- c(correlationName,paste(var1,":",entity))
            if(corVal > 0){
                correlationSign <- c(correlationSign,"+ve Correlation")
            }
            else{
                correlationSign <- c(correlationSign,"-ve Correlation")
            }
            absoluteCorrelationValue <-␣
 ↪c(absoluteCorrelationValue,abs(cor(data[var1],data[entity])))
        }
    }
}
temp = data.
 ↪frame(correlationName,correlationValues,absoluteCorrelationValue,correlationSign)
newCorrelation = temp[order(-temp$absoluteCorrelationValue),]
newCorrelation
```

	correlationName	correlationValues	absoluteCorrelatio
10	entropy_fie : entropy_atomic_radius	0.9977394	0.9977394
82	wtd_mean_Valence : wtd_gmean_Valence	0.9949388	0.9949388
19	entropy_Valence : entropy_fie	0.9927256	0.9927256
43	mean_Valence : gmean_Valence	0.9899105	0.9899105
12	entropy_Valence : entropy_atomic_radius	0.9895461	0.9895461
64	std_ThermalConductivity : range_ThermalConductivity	0.9878666	0.9878666
60	std_fie : range_fie	0.9816283	0.9816283
20	number_of_elements : entropy_fie	0.9731953	0.9731953
1	entropy_atomic_radius : entropy_atomic_mass	0.9723288	0.9723288
13	number_of_elements : entropy_atomic_radius	0.9722452	0.9722452
31	number_of_elements : entropy_Valence	0.9678325	0.9678325
53	std_atomic_radius : range_atomic_radius	0.9674282	0.9674282
65	wtd_std_ThermalConductivity : range_ThermalConductivity	0.9654488	0.9654488
2	entropy_fie : entropy_atomic_mass	0.9646946	0.9646946
4	entropy_Valence : entropy_atomic_mass	0.9636211	0.9636211
72	wtd_entropy_atomic_radius : wtd_entropy_atomic_mass	0.9614639	0.9614639
57	wtd_std_atomic_radius : range_atomic_radius	0.9580035	0.9580035
71	wtd_std_ThermalConductivity : std_ThermalConductivity	0.9556271	0.9556271
42	wtd_gmean_Density : gmean_Density	0.9519949	0.9519949
76	wtd_entropy_Valence : wtd_entropy_atomic_radius	0.9514635	0.9514635
67	wtd_std_atomic_radius : std_atomic_radius	0.9445362	0.9445362
63	wtd_std_fie : range_fie	0.9402813	0.9402813
46	wtd_gmean_Valence : mean_Valence	0.9400013	0.9400013
5	number_of_elements : entropy_atomic_mass	0.9393041	0.9393041
47	wtd_mean_Valence : mean_Valence	0.9371029	0.9371029
70	wtd_std_fie : std_fie	0.9342550	0.9342550
44	wtd_gmean_Valence : gmean_Valence	0.9330357	0.9330357
11	entropy_FusionHeat : entropy_atomic_radius	0.9302940	0.9302940
3	entropy_FusionHeat : entropy_atomic_mass	0.9282509	0.9282509
83	wtd_std_fie : wtd_std_atomic_radius	0.9222584	0.9222584
...	...	...	...
29	wtd_entropy_FusionHeat : entropy_FusionHeat	0.8816549	0.8816549
7	wtd_entropy_atomic_radius : entropy_atomic_mass	0.8802129	0.8802129
66	std_fie : std_atomic_radius	0.8760793	0.8760793
73	wtd_entropy_FusionHeat : wtd_entropy_atomic_mass	0.8739307	0.8739307
62	wtd_std_atomic_radius : range_fie	0.8717110	0.8717110
16	wtd_entropy_FusionHeat : entropy_atomic_radius	0.8674232	0.8674232
34	wtd_entropy_FusionHeat : entropy_Valence	0.8660684	0.8660684
59	std_atomic_radius : range_fie	0.8646203	0.8646203
23	wtd_entropy_FusionHeat : entropy_fie	0.8642142	0.8642142
9	wtd_entropy_Valence : entropy_atomic_mass	0.8614787	0.8614787
50	wtd_entropy_FusionHeat : number_of_elements	0.8604788	0.8604788
69	wtd_std_atomic_radius : std_fie	0.8590586	0.8590586
8	wtd_entropy_FusionHeat : entropy_atomic_mass	0.8450895	0.8450895
68	wtd_std_fie : std_atomic_radius	0.8444218	0.8444218
28	wtd_entropy_atomic_radius : entropy_FusionHeat	0.8411200	0.8411200
27	wtd_entropy_atomic_mass : entropy_FusionHeat	0.8350191	0.8350191
36	gmean_Valence : gmean_Density	0.8295007	0.8295007
80	wtd_std_atomic_radius : wtd_gmean_Density	-0.8288245	0.8288245
81	wtd_std_fie : wtd_gmean_Density	-0.8252281	0.8252281
30	wtd_entropy_Valence : entropy_FusionHeat	0.8241210	0.8241210
56	wtd_gmean_Density : range_atomic_radius	-0.8173336	0.8173336

[20]:
```
print(paste("So there is about",nrow(newCorrelation),"entries with correlation␣
↪greater than abs(0.8)"))
```

```
[1] "So there is about 83 entries with correlation greater than abs(0.8)"
```

[21]:
```
newCorrelation99 = newCorrelation[newCorrelation$absoluteCorrelationValue > 0.
↪99,]
newCorrelation99
```

	correlationName	correlationValues	absoluteCorrelationValue	correlation
10	entropy_fie : entropy_atomic_radius	0.9977394	0.9977394	+ve Corre
82	wtd_mean_Valence : wtd_gmean_Valence	0.9949388	0.9949388	+ve Corre
19	entropy_Valence : entropy_fie	0.9927256	0.9927256	+ve Corre

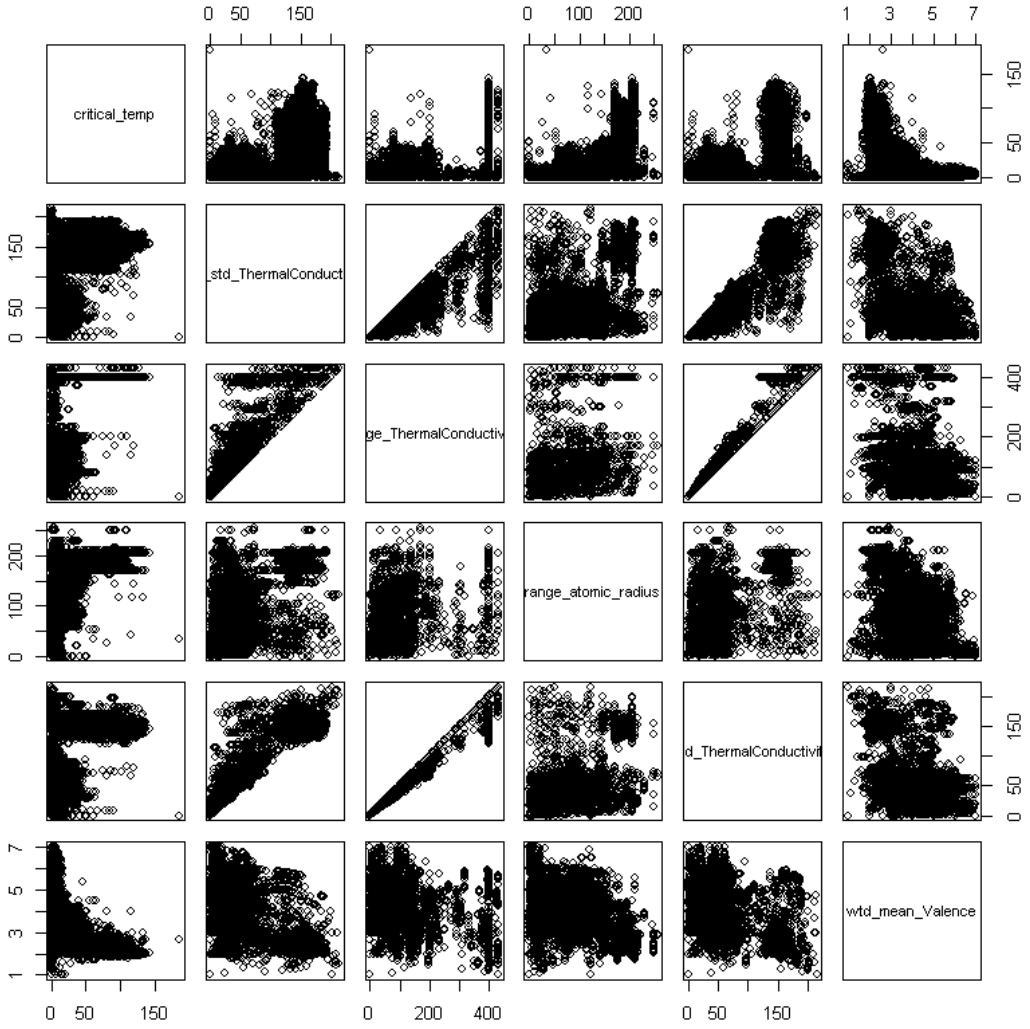
[22]:
```
print(paste("So there is about",nrow(newCorrelation99),"entries with␣
↪correlation greater than abs(0.99)"))
```

```
[1] "So there is about 3 entries with correlation greater than abs(0.99)"
```

3.1.2 Individual Analysis of Top 5 Correlated Variables

[115]:
```
top5Columns =␣
↪c('critical_temp','wtd_std_ThermalConductivity','range_ThermalConductivity','range_atomic_r
                'std_ThermalConductivity','wtd_mean_Valence')
top5ColumnsData = data[,top5Columns]
```

[116]:
```
pairs(top5ColumnsData)
```

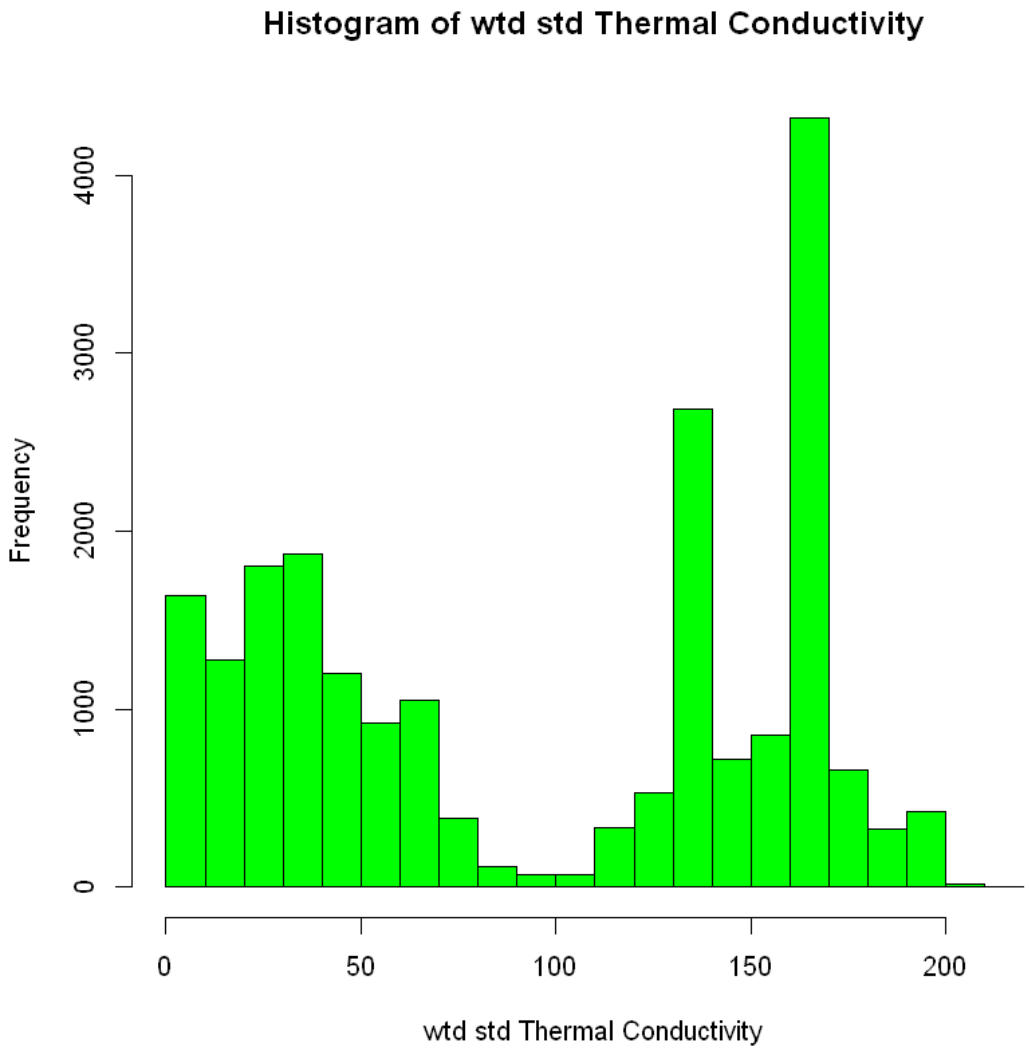


From the above plot we can see that some of the columns are linearly correlated to each other

3.1.3 Checking the internal splitup of the top 5 correlated predictors

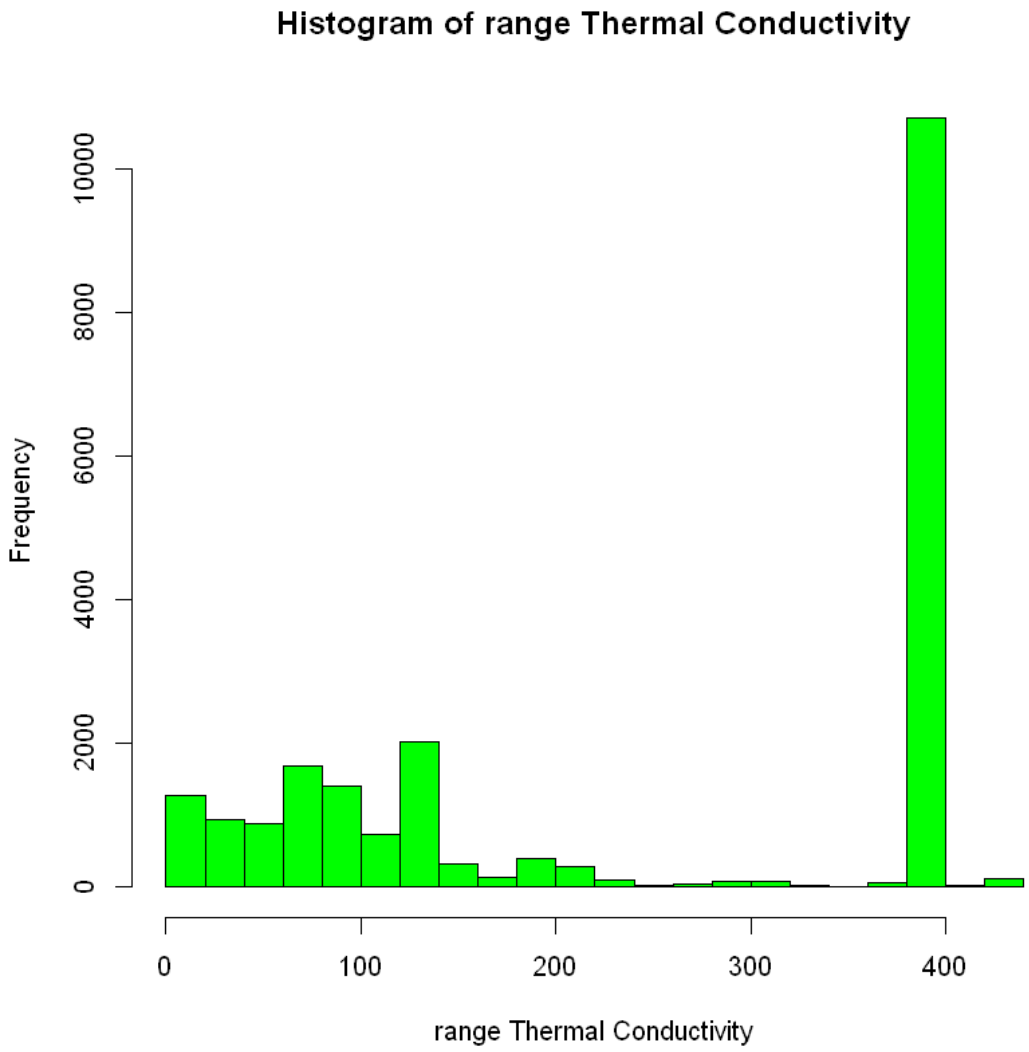
3.1.4 wtd Std Thermal Conductivity

[23]:
```
hist(data$wtd_std_ThermalConductivity,col="green",xlab ="wtd std Thermal␣
↪Conductivity" ,
    main="Histogram of wtd std Thermal Conductivity")
```



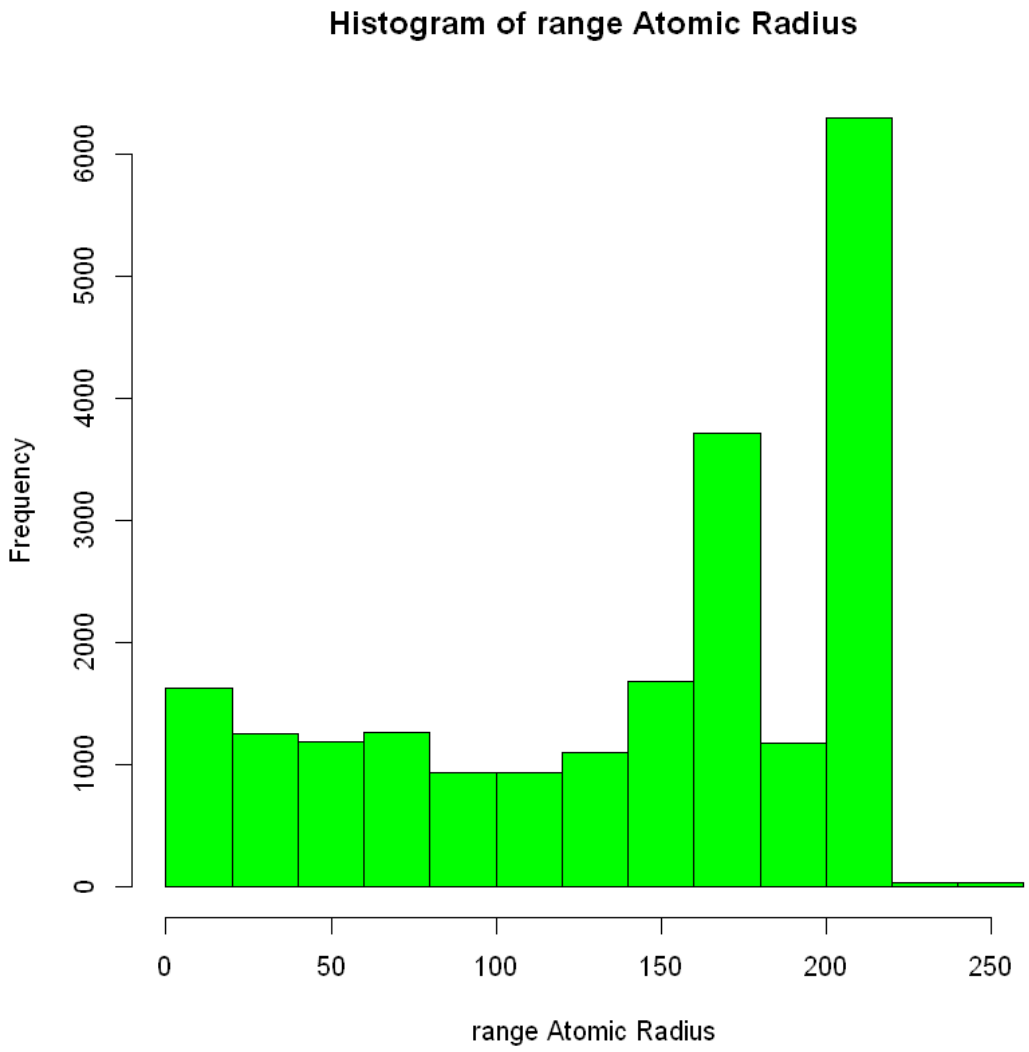
3.1.5 range Thermal Conductivity

[24]:
```
hist(data$range_ThermalConductivity,col="green",xlab ="range Thermal␣
↪Conductivity" ,
    main="Histogram of range Thermal Conductivity")
```



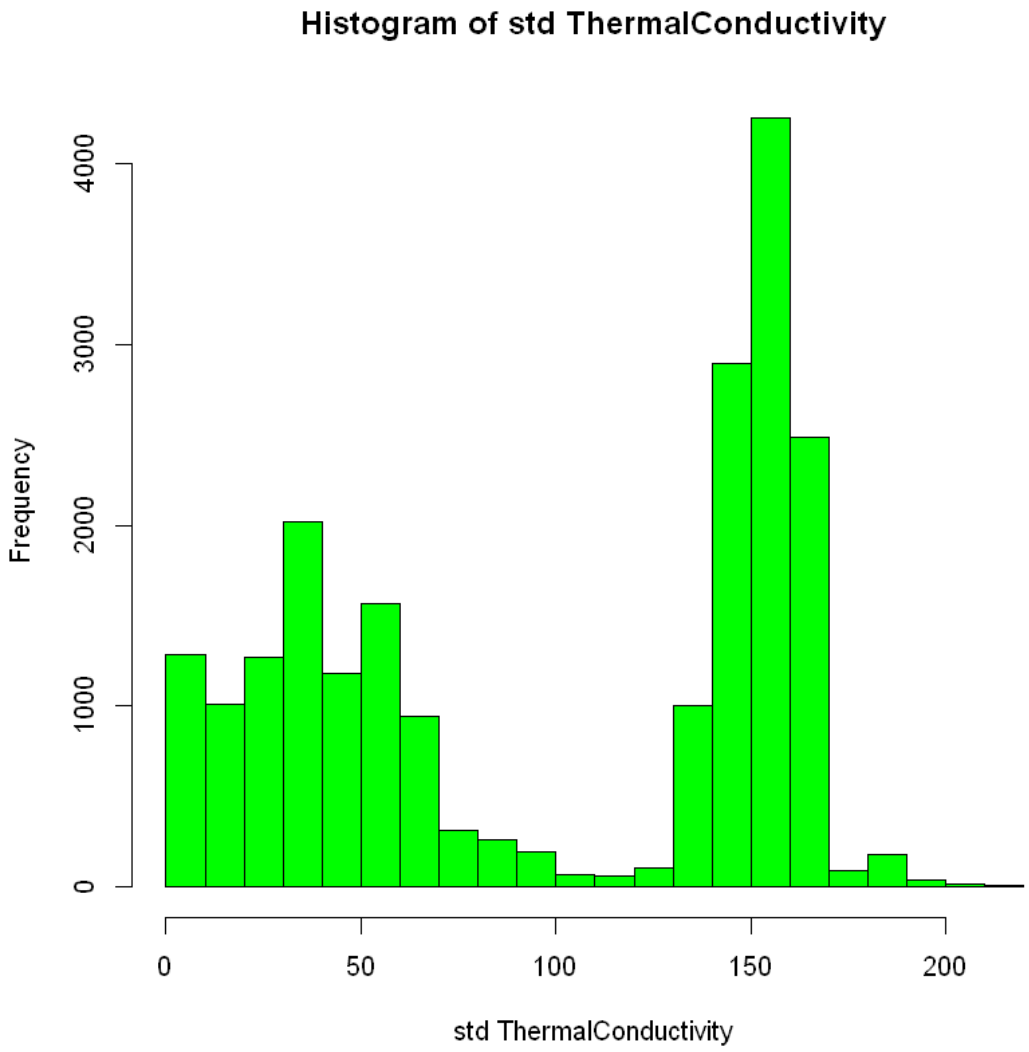
3.1.6 range atomic radius

[25]:
```
hist(data$range_atomic_radius,col="green",xlab ="range Atomic Radius" ,
     main="Histogram of range Atomic Radius")
```



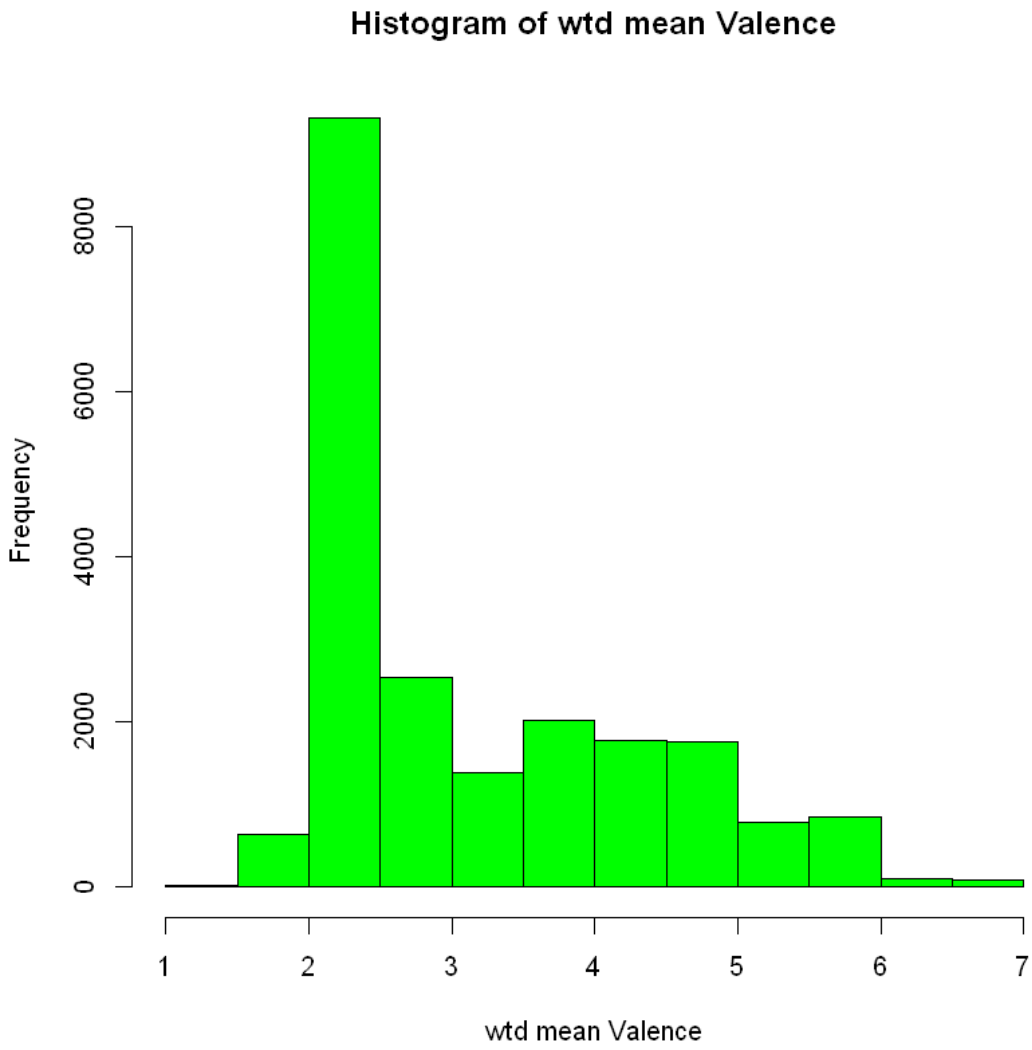
3.1.7 std_ThermalConductivity

[26]:
```
hist(data$std_ThermalConductivity,col="green",xlab ="std ThermalConductivity" ,
     main="Histogram of std ThermalConductivity")
```



3.1.8 wtd_mean_Valence

[27]:
```
hist(data$wtd_mean_Valence,col="green",xlab ="wtd mean Valence" ,
     main="Histogram of wtd mean Valence")
```



4 Models

4.1 Splitting Data into Training and Test Data

[28]:
```
#Splitting the data into 70 percent training and 30 percent test data
sampleSize <- floor(0.70 * nrow(data))

## set the seed to make your partition reproducible
set.seed(123)
trainIndex <- sample(seq_len(nrow(data)), size = sampleSize)
train <- data[trainIndex, ]
test <- data[-trainIndex, ]
```

Checking train data

[29]:
```
describe(train)
```

	vars	n	mean	sd	median	trimmed
number_of_elements	1	14884	4.1158291	1.4396949	4.0000000	4.1051394
mean_atomic_mass	2	14884	87.3647050	29.5389742	84.8135000	85.7441299
wtd_mean_atomic_mass	3	14884	72.6897101	33.1898236	60.6300009	68.2818970
gmean_atomic_mass	4	14884	71.1173843	30.8033251	66.3615924	67.5347268
wtd_gmean_atomic_mass	5	14884	58.2686201	36.3175172	39.7293639	51.9595490
entropy_atomic_mass	6	14884	1.1660909	0.3650778	1.1995407	1.1929022
wtd_entropy_atomic_mass	7	14884	1.0635837	0.4008431	1.1426027	1.0922855
range_atomic_mass	8	14884	115.5605139	54.5695196	122.9060700	118.665737
wtd_range_atomic_mass	9	14884	33.0425770	26.4968561	26.7171854	28.6455916
std_atomic_mass	10	14884	44.3796910	20.0130003	45.1235000	45.3059567
wtd_std_atomic_mass	11	14884	41.3966476	19.9624902	44.2859836	42.0127606
mean_fie	12	14884	768.9138352	86.9125185	763.5595238	762.389261
wtd_mean_fie	13	14884	870.0029323	143.3459768	889.5260000	878.486953
gmean_fie	14	14884	736.8573559	77.8765660	727.8459992	729.535320
wtd_gmean_fie	15	14884	832.3712924	119.7961487	855.1594887	839.009672
entropy_fie	16	14884	1.2995259	0.3814259	1.3544667	1.3253022
wtd_entropy_fie	17	14884	0.9258569	0.3327233	0.9162367	0.9230587
range_fie	18	14884	571.4061072	308.8721318	764.1000000	592.452099
wtd_range_fie	19	14884	484.1411264	223.4130049	511.7731000	495.641947
std_fie	20	14884	215.3368425	109.7596713	265.9993907	221.388392
wtd_std_fie	21	14884	223.8115507	127.9707376	257.7482760	232.762299
mean_atomic_radius	22	14884	157.9899346	20.0664920	160.2500000	159.053182
wtd_mean_atomic_radius	23	14884	134.6460460	28.8233118	125.8744592	132.267944
gmean_atomic_radius	24	14884	144.4673042	21.9844730	142.9395477	144.285235
wtd_gmean_atomic_radius	25	14884	120.9277770	35.8159632	113.1700600	117.504696
entropy_atomic_radius	26	14884	1.2681924	0.3751280	1.3295198	1.2921974
wtd_entropy_atomic_radius	27	14884	1.1307925	0.4059713	1.2403342	1.1667264
range_atomic_radius	28	14884	139.4197124	67.0592191	171.0000000	146.904098
wtd_range_atomic_radius	29	14884	51.3150776	34.8515944	43.2000000	45.7057959
std_atomic_radius	30	14884	51.6173240	22.7905834	58.6562870	53.7939542
...	...	...	...	...	...	...
wtd_mean_FusionHeat	53	14884	13.9043695	14.3249444	8.3471667	11.0021963
gmean_FusionHeat	54	14884	10.1774573	10.1073960	5.2732622	8.1942707
wtd_gmean_FusionHeat	55	14884	10.2002350	13.1777367	4.9501473	7.6862900
entropy_FusionHeat	56	14884	1.0946401	0.3760006	1.1120982	1.1152976
wtd_entropy_FusionHeat	57	14884	0.9133378	0.3699848	0.9947607	0.9366544
range_FusionHeat	58	14884	21.1549454	20.3213094	12.8780000	16.9259227
wtd_range_FusionHeat	59	14884	8.2738365	11.4496698	3.4435000	5.9457891
std_FusionHeat	60	14884	8.3289602	8.6478381	4.9481553	6.3956365
wtd_std_FusionHeat	61	14884	7.7314884	7.2993587	5.4940314	6.2431409
mean_ThermalConductivity	62	14884	90.0145070	38.4783166	96.6053160	90.2502107
wtd_mean_ThermalConductivity	63	14884	81.8351752	45.5846014	73.4970880	77.1714687
gmean_ThermalConductivity	64	14884	29.9823930	34.1750426	14.4204935	23.1704014
wtd_gmean_ThermalConductivity	65	14884	27.4804875	40.2419595	6.1377658	19.2998938
entropy_ThermalConductivity	66	14884	0.7286779	0.3264014	0.7413766	0.7319282
wtd_entropy_ThermalConductivity	67	14884	0.5398728	0.3181558	0.5448699	0.5232617
range_ThermalConductivity	68	14884	251.6052819	158.5130421	399.8964600	262.162768
wtd_range_ThermalConductivity	69	14884	62.2439172	43.0738024	56.5562400	57.9657323
std_ThermalConductivity	70	14884	99.2280091	60.0776163	135.7822792	101.620846
wtd_std_ThermalConductivity	71	14884	96.4820210	63.6133250	115.1813787	97.6344224
mean_Valence	72	14884	3.1924361	1.0422309	2.8333333	3.0541121
wtd_mean_Valence	73	14884	3.1480182	1.1875890	2.6088665	2.9875715

4.1.1 Initially we will check with all the predictors

[30]:
```
fit.all = lm(critical_temp~., data = train)
fit.all.summary = summary(fit.all)
fit.all.summary
```

```
Call:
lm(formula = critical_temp ~ ., data = train)

Residuals:
    Min      1Q  Median      3Q     Max
-84.935  -9.388   0.552  10.893 169.773

Coefficients:
                                Estimate Std. Error t value Pr(>|t|)
(Intercept)                   -2.372e+01  6.009e+00  -3.947 7.94e-05 ***
number_of_elements            -3.068e+00  8.944e-01  -3.430 0.000605 ***
mean_atomic_mass               8.091e-01  9.915e-02   8.160 3.61e-16 ***
wtd_mean_atomic_mass          -8.319e-01  1.241e-01  -6.704 2.10e-11 ***
gmean_atomic_mass             -4.412e-01  9.838e-02  -4.485 7.35e-06 ***
wtd_gmean_atomic_mass          5.487e-01  1.179e-01   4.653 3.29e-06 ***
entropy_atomic_mass           -3.890e+01  5.467e+00  -7.116 1.16e-12 ***
wtd_entropy_atomic_mass        6.834e+00  4.328e+00   1.579 0.114373
range_atomic_mass              2.181e-01  1.979e-02  11.018  < 2e-16 ***
wtd_range_atomic_mass          3.634e-02  2.645e-02   1.374 0.169497
std_atomic_mass               -5.844e-01  7.575e-02  -7.715 1.29e-14 ***
wtd_std_atomic_mass            9.650e-02  6.578e-02   1.467 0.142396
mean_fie                       2.028e-01  7.605e-02   2.667 0.007668 **
wtd_mean_fie                  -2.402e-01  9.241e-02  -2.599 0.009363 **
gmean_fie                     -2.002e-01  7.510e-02  -2.665 0.007702 **
wtd_gmean_fie                  2.671e-01  9.124e-02   2.927 0.003426 **
entropy_fie                   -1.287e+02  2.404e+01  -5.352 8.85e-08 ***
wtd_entropy_fie                4.746e+01  5.699e+00   8.328  < 2e-16 ***
range_fie                      6.762e-02  7.794e-03   8.675  < 2e-16 ***
wtd_range_fie                  2.396e-02  4.352e-03   5.504 3.77e-08 ***
std_fie                       -2.021e-01  2.681e-02  -7.538 5.04e-14 ***
wtd_std_fie                   -1.688e-02  2.461e-02  -0.686 0.492714
mean_atomic_radius            -4.474e-01  2.167e-01  -2.065 0.038957 *
wtd_mean_atomic_radius         3.066e+00  2.879e-01  10.649  < 2e-16 ***
gmean_atomic_radius            1.076e-01  2.173e-01   0.495 0.620577
wtd_gmean_atomic_radius       -2.660e+00  2.822e-01  -9.427  < 2e-16 ***
entropy_atomic_radius          8.350e+01  2.109e+01   3.959 7.55e-05 ***
wtd_entropy_atomic_radius      3.895e+01  6.343e+00   6.140 8.47e-10 ***
range_atomic_radius            2.091e-01  2.663e-02   7.851 4.41e-15 ***
wtd_range_atomic_radius       -9.686e-02  1.913e-02  -5.063 4.18e-07 ***
std_atomic_radius             -4.464e-01  1.177e-01  -3.793 0.000149 ***
wtd_std_atomic_radius         -2.427e-01  1.048e-01  -2.317 0.020514 *
mean_Density                  -4.983e-03  5.982e-04  -8.330  < 2e-16 ***
```

```
wtd_mean_Density                -1.144e-04  7.342e-04  -0.156 0.876195
gmean_Density                    1.190e-03  5.673e-04   2.097 0.036035 *
wtd_gmean_Density                2.377e-03  7.042e-04   3.376 0.000738 ***
entropy_Density                  1.638e+01  4.146e+00   3.952 7.78e-05 ***
wtd_entropy_Density             -1.986e+01  3.201e+00  -6.204 5.63e-10 ***
range_Density                   -1.740e-03  2.576e-04  -6.754 1.49e-11 ***
wtd_range_Density               -2.215e-05  3.124e-04  -0.071 0.943467
std_Density                      6.618e-03  8.347e-04   7.928 2.38e-15 ***
wtd_std_Density                 -1.759e-03  6.141e-04  -2.864 0.004194 **
mean_ElectronAffinity           -7.261e-02  5.584e-02  -1.300 0.193483
wtd_mean_ElectronAffinity        4.889e-01  6.074e-02   8.049 9.00e-16 ***
gmean_ElectronAffinity           1.351e-01  4.846e-02   2.788 0.005316 **
wtd_gmean_ElectronAffinity      -5.283e-01  5.360e-02  -9.857  < 2e-16 ***
entropy_ElectronAffinity         5.553e+00  3.097e+00   1.793 0.073014 .
wtd_entropy_ElectronAffinity    -2.445e+01  2.642e+00  -9.254  < 2e-16 ***
range_ElectronAffinity          -3.794e-01  2.096e-02 -18.102  < 2e-16 ***
wtd_range_ElectronAffinity      -1.604e-01  2.502e-02  -6.413 1.47e-10 ***
std_ElectronAffinity             1.246e+00  6.993e-02  17.818  < 2e-16 ***
wtd_std_ElectronAffinity        -5.234e-01  4.694e-02 -11.149  < 2e-16 ***
mean_FusionHeat                  1.661e+00  2.257e-01   7.356 1.99e-13 ***
wtd_mean_FusionHeat             -1.924e+00  2.310e-01  -8.328  < 2e-16 ***
gmean_FusionHeat                -1.433e+00  2.054e-01  -6.975 3.20e-12 ***
wtd_gmean_FusionHeat             1.526e+00  2.127e-01   7.175 7.57e-13 ***
entropy_FusionHeat              -1.832e+01  3.304e+00  -5.545 3.00e-08 ***
wtd_entropy_FusionHeat           2.578e+01  2.316e+00  11.134  < 2e-16 ***
range_FusionHeat                -3.755e-01  8.024e-02  -4.679 2.91e-06 ***
wtd_range_FusionHeat             6.611e-01  8.154e-02   8.108 5.56e-16 ***
std_FusionHeat                  -4.655e-01  3.141e-01  -1.482 0.138430
wtd_std_FusionHeat               6.671e-01  1.874e-01   3.560 0.000372 ***
mean_ThermalConductivity        -5.480e-02  2.943e-02  -1.862 0.062625 .
wtd_mean_ThermalConductivity     5.287e-01  3.355e-02  15.761  < 2e-16 ***
gmean_ThermalConductivity       -6.439e-02  2.781e-02  -2.315 0.020630 *
wtd_gmean_ThermalConductivity   -3.346e-01  3.203e-02 -10.447  < 2e-16 ***
entropy_ThermalConductivity      1.049e+01  2.374e+00   4.419 9.99e-06 ***
wtd_entropy_ThermalConductivity  2.419e+00  1.907e+00   1.268 0.204813
range_ThermalConductivity       -9.520e-02  1.589e-02  -5.992 2.12e-09 ***
wtd_range_ThermalConductivity   -2.225e-01  1.964e-02 -11.332  < 2e-16 ***
std_ThermalConductivity          2.977e-01  4.917e-02   6.053 1.46e-09 ***
wtd_std_ThermalConductivity     -2.162e-02  2.726e-02  -0.793 0.427612
mean_Valence                    -1.740e+01  7.291e+00  -2.386 0.017032 *
wtd_mean_Valence                 2.846e+01  8.743e+00   3.255 0.001136 **
gmean_Valence                    2.155e+01  6.887e+00   3.130 0.001752 **
wtd_gmean_Valence               -3.244e+01  8.201e+00  -3.956 7.65e-05 ***
entropy_Valence                  7.956e+01  1.473e+01   5.402 6.70e-08 ***
wtd_entropy_Valence             -6.711e+01  6.685e+00 -10.039  < 2e-16 ***
range_Valence                    5.718e+00  8.828e-01   6.477 9.64e-11 ***
wtd_range_Valence               -9.108e-01  7.627e-01  -1.194 0.232436
std_Valence                      6.026e+00  2.950e+00   2.043 0.041067 *
```

```
wtd_std_Valence                -2.694e+01  2.296e+00 -11.735  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.62 on 14802 degrees of freedom
Multiple R-squared:  0.7369,Adjusted R-squared:  0.7355
F-statistic: 511.9 on 81 and 14802 DF,  p-value: < 2.2e-16
```

[31]:
```
print(paste("Adjusted R-Square:",round(fit.all.summary$adj.r.squared,4)))
```

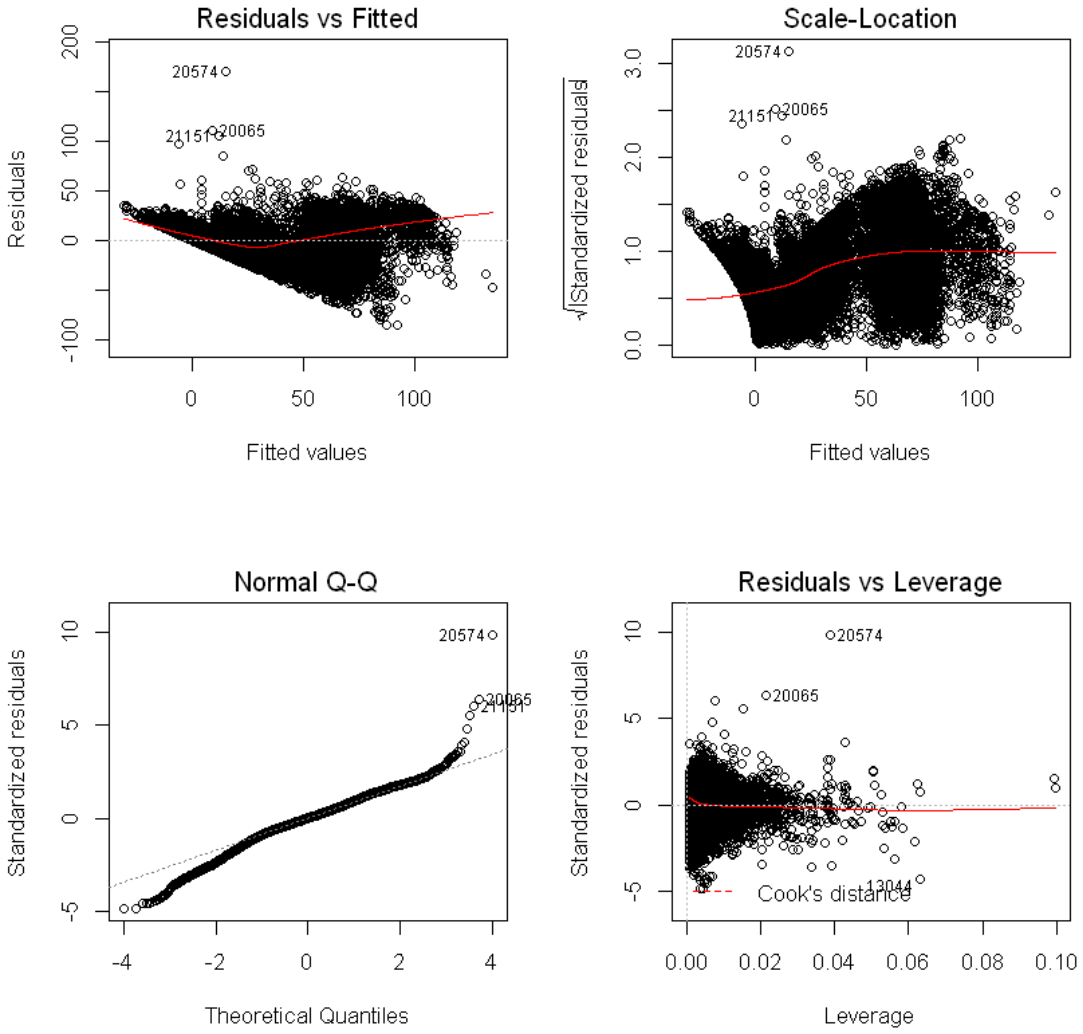
```
[1] "Adjusted R-Square: 0.7355"
```

[32]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.all.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 81 predictors is been used"
```

Lets Check the various Residuals plot

[33]:
```
par(mfcol=c(2,2))
plot(fit.all)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if

residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.2 Linear FIt just based on the columns Which have higher correlation that is greater than 0.5 or less than -0.5

[34]:
```
levels(correlation$correlationName)
```

1. 'critical_temp' 2. 'entropy_atomic_mass' 3. 'entropy_atomic_radius' 4. 'entropy_fie' 5. 'entropy_FusionHeat' 6. 'entropy_Valence' 7. 'gmean_Density' 8. 'gmean_Valence' 9. 'mean_Valence' 10. 'number_of_elements' 11. 'range_atomic_radius' 12. 'range_fie' 13. 'range_ThermalConductivity' 14. 'std_atomic_radius' 15. 'std_fie' 16. 'std_ThermalConductivity' 17. 'wtd_entropy_atomic_mass' 18. 'wtd_entropy_atomic_radius' 19. 'wtd_entropy_FusionHeat' 20. 'wtd_entropy_Valence' 21. 'wtd_gmean_Density' 22. 'wtd_gmean_Valence' 23. 'wtd_mean_Valence' 24. 'wtd_std_atomic_radius' 25. 'wtd_std_fie' 26. 'wtd_std_ThermalConductivity'

[35]:
```
newTrain = train[,levels(correlation$correlationName)]
describe(newTrain)
```

	vars	n	mean	sd	median	trimmed
critical_temp	1	14884	34.4200738	34.2579981	20.0000000	30.2936453
entropy_atomic_mass	2	14884	1.1660909	0.3650778	1.1995407	1.1929022
entropy_atomic_radius	3	14884	1.2681924	0.3751280	1.3295198	1.2921974
entropy_fie	4	14884	1.2995259	0.3814259	1.3544667	1.3253022
entropy_FusionHeat	5	14884	1.0946401	0.3760006	1.1120982	1.1152976
entropy_Valence	6	14884	1.2961217	0.3929598	1.3689224	1.3231384
gmean_Density	7	14884	3455.0483931	3688.0210618	1339.9747016	2830.811650
gmean_Valence	8	14884	3.0514286	1.0436272	2.6153210	2.8966508
mean_Valence	9	14884	3.1924361	1.0422309	2.8333333	3.0541121
number_of_elements	10	14884	4.1158291	1.4396949	4.0000000	4.1051394
range_atomic_radius	11	14884	139.4197124	67.0592191	171.0000000	146.9040981
range_fie	12	14884	571.4061072	308.8721318	764.1000000	592.4520994
range_ThermalConductivity	13	14884	251.6052819	158.5130421	399.8964600	262.1627682
std_atomic_radius	14	14884	51.6173240	22.7905834	58.6562870	53.7939542
std_fie	15	14884	215.3368425	109.7596713	265.9993907	221.3883928
std_ThermalConductivity	16	14884	99.2280091	60.0776163	135.7822792	101.6208461
wtd_entropy_atomic_mass	17	14884	1.0635837	0.4008431	1.1426027	1.0922855
wtd_entropy_atomic_radius	18	14884	1.1307925	0.4059713	1.2403342	1.1667264
wtd_entropy_FusionHeat	19	14884	0.9133378	0.3699848	0.9947607	0.9366544
wtd_entropy_Valence	20	14884	1.0519782	0.3794388	1.1550007	1.0823027
wtd_gmean_Density	21	14884	3105.2285976	3948.0348627	1537.5539857	2428.192483
wtd_gmean_Valence	22	14884	3.0508850	1.1712056	2.4319843	2.8760842
wtd_mean_Valence	23	14884	3.1480182	1.1875890	2.6088665	2.9875715
wtd_std_atomic_radius	24	14884	52.3487934	25.2058855	60.1706052	54.7417064
wtd_std_fie	25	14884	223.8115507	127.9707376	257.7482760	232.7622994
wtd_std_ThermalConductivity	26	14884	96.4820210	63.6133250	115.1813787	97.6344224

[36]:
```
fit.correlated = lm(critical_temp~., data = newTrain)
fit.correlated.summary = summary(fit.correlated)
fit.correlated.summary
```

```
Call:
lm(formula = critical_temp ~ ., data = newTrain)

Residuals:
    Min      1Q  Median      3Q     Max
-82.676 -12.678   0.126  12.752 190.625

Coefficients:
                           Estimate Std. Error t value Pr(>|t|)
(Intercept)                2.794e+01  1.703e+00  16.404  < 2e-16 ***
entropy_atomic_mass       -6.009e+01  2.584e+00 -23.257  < 2e-16 ***
entropy_atomic_radius     -3.559e+01  1.520e+01  -2.342  0.01919 *
entropy_fie                1.306e+02  1.749e+01   7.467 8.68e-14 ***
entropy_FusionHeat         9.827e+00  2.067e+00   4.753 2.02e-06 ***
entropy_Valence           -6.518e+01  1.302e+01  -5.006 5.61e-07 ***
gmean_Density             -3.850e-03  2.074e-04 -18.567  < 2e-16 ***
```

```
gmean_Valence                1.741e+01  4.629e+00   3.760  0.00017 ***
mean_Valence                -1.791e+01  4.631e+00  -3.868  0.00011 ***
number_of_elements          -4.477e+00  8.464e-01  -5.290 1.24e-07 ***
range_atomic_radius          5.441e-01  2.622e-02  20.748  < 2e-16 ***
range_fie                    5.503e-02  7.261e-03   7.578 3.71e-14 ***
range_ThermalConductivity    2.268e-02  1.553e-02   1.461  0.14415
std_atomic_radius           -1.512e+00  7.321e-02 -20.658  < 2e-16 ***
std_fie                      3.011e-03  1.963e-02   0.153  0.87812
std_ThermalConductivity     -1.890e-01  3.435e-02  -5.502 3.82e-08 ***
wtd_entropy_atomic_mass      5.543e+01  2.157e+00  25.696  < 2e-16 ***
wtd_entropy_atomic_radius   -1.611e+01  3.225e+00  -4.996 5.93e-07 ***
wtd_entropy_FusionHeat       1.351e+01  1.645e+00   8.213 2.32e-16 ***
wtd_entropy_Valence         -2.960e+01  2.394e+00 -12.364  < 2e-16 ***
wtd_gmean_Density            3.268e-03  1.935e-04  16.889  < 2e-16 ***
wtd_gmean_Valence            3.356e+01  3.366e+00   9.970  < 2e-16 ***
wtd_mean_Valence            -3.509e+01  3.341e+00 -10.501  < 2e-16 ***
wtd_std_atomic_radius        3.108e-01  4.643e-02   6.693 2.27e-11 ***
wtd_std_fie                 -1.179e-01  9.502e-03 -12.405  < 2e-16 ***
wtd_std_ThermalConductivity  3.190e-01  1.239e-02  25.749  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 20.38 on 14858 degrees of freedom
Multiple R-squared:  0.6467,Adjusted R-squared:  0.6461
F-statistic:  1088 on 25 and 14858 DF,  p-value: < 2.2e-16
```

[37]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.all.summary$adj.r.
 ↪squared,4)))
print(paste("Highly Correlated Data - Adjusted R-Square:",round(fit.correlated.
 ↪summary$adj.r.squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7355"
[1] "Highly Correlated Data - Adjusted R-Square: 0.6461"
```

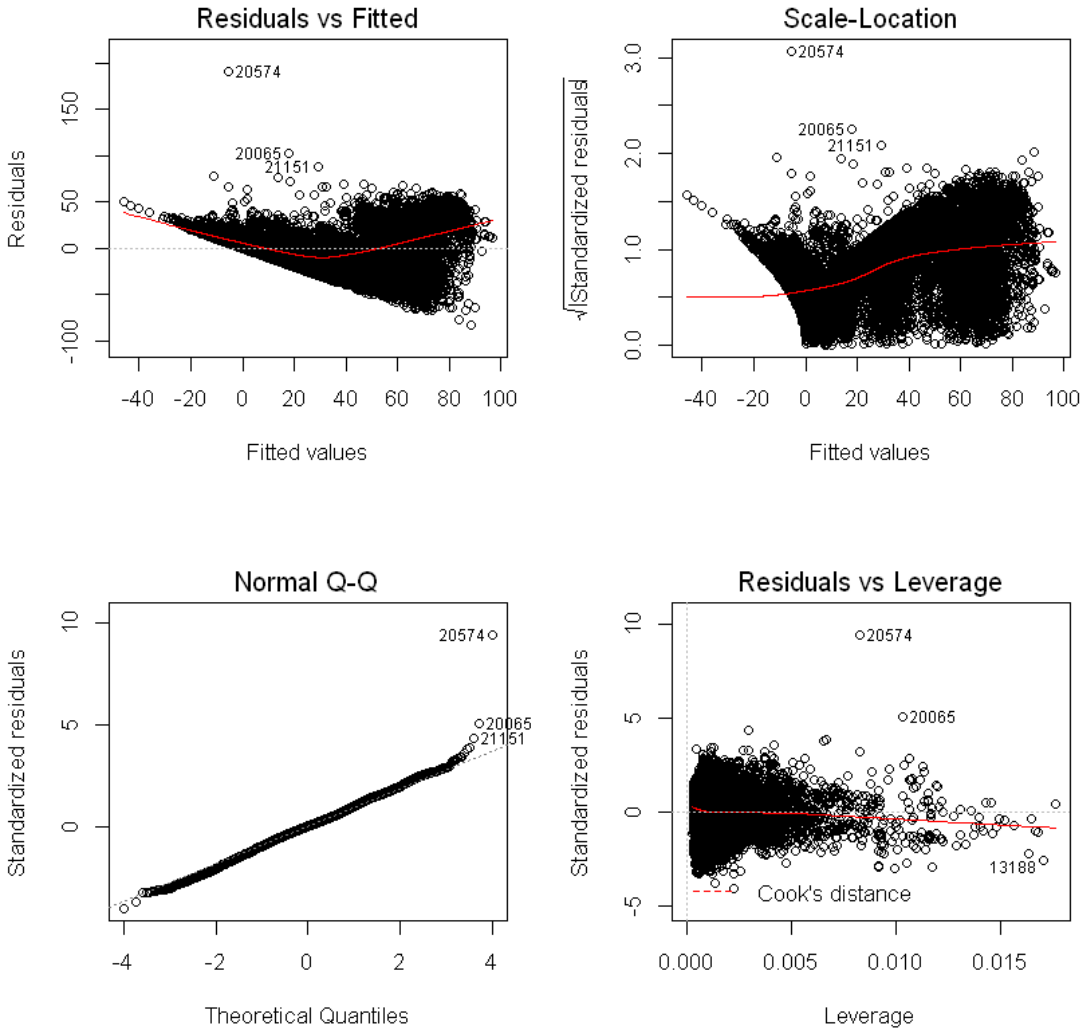
Here we can see that the Adjusted R square has been reduced significantly Which indicates the new model might not be a good model

[38]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.correlated.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 25 predictors is been used"
```

Lets Check the various Residuals plot

[39]:
```
par(mfcol=c(2,2))
plot(fit.correlated)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if

residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.3 Perform F-tests by comparing the two models using the anova() function

[40]:
```
anova(fit.all, fit.correlated)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14858	6170995	-56	-1576097	90.66492	0

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are more correlated as p value is 0. we can also see that in the new fit there is predictors less compared to the original which makes it less complex. But we also see that RSS value has been increased significantly which is very bad.

Trying to Add the top 3 inter correlated columns that we found earlier and checking its adjusted rsquare val

[117]:
```
summary(update(fit.correlated, . ~ . + entropy_fie:entropy_atomic_radius +␣
↪wtd_mean_Valence:wtd_gmean_Valence + entropy_Valence:entropy_fie))
```

```
Call:
lm(formula = critical_temp ~ entropy_atomic_mass + entropy_atomic_radius +
    entropy_fie + entropy_FusionHeat + entropy_Valence + gmean_Density +
    gmean_Valence + mean_Valence + number_of_elements + range_atomic_radius +
    range_fie + range_ThermalConductivity + std_atomic_radius +
    std_fie + std_ThermalConductivity + wtd_entropy_atomic_mass +
    wtd_entropy_atomic_radius + wtd_entropy_FusionHeat + wtd_entropy_Valence +
    wtd_gmean_Density + wtd_gmean_Valence + wtd_mean_Valence +
    wtd_std_atomic_radius + wtd_std_fie + wtd_std_ThermalConductivity +
    entropy_atomic_radius:entropy_fie + wtd_gmean_Valence:wtd_mean_Valence +
    entropy_fie:entropy_Valence, data = newTrain)

Residuals:
```

```
    Min      1Q  Median      3Q     Max
-83.726 -12.302  -0.029  12.618 200.864

Coefficients:
                                    Estimate Std. Error t value Pr(>|t|)
(Intercept)                         4.213e+01  4.619e+00   9.120  < 2e-16 ***
entropy_atomic_mass                -5.616e+01  2.569e+00 -21.861  < 2e-16 ***
entropy_atomic_radius              -1.999e+02  2.108e+01  -9.483  < 2e-16 ***
entropy_fie                         4.736e+01  1.795e+01   2.638  0.00836 **
entropy_FusionHeat                  9.889e+00  2.063e+00   4.794 1.65e-06 ***
entropy_Valence                     1.948e+02  2.351e+01   8.285  < 2e-16 ***
gmean_Density                      -3.419e-03  2.066e-04 -16.551  < 2e-16 ***
gmean_Valence                       3.270e+00  4.737e+00   0.690  0.49003
mean_Valence                       -6.385e+00  4.712e+00  -1.355  0.17545
number_of_elements                  1.882e+01  2.605e+00   7.224 5.30e-13 ***
range_atomic_radius                 5.723e-01  2.640e-02  21.674  < 2e-16 ***
range_fie                           6.058e-02  7.268e-03   8.335  < 2e-16 ***
range_ThermalConductivity           2.882e-02  1.553e-02   1.856  0.06349 .
std_atomic_radius                  -1.629e+00  7.411e-02 -21.980  < 2e-16 ***
std_fie                            -3.824e-02  1.986e-02  -1.925  0.05425 .
std_ThermalConductivity            -2.031e-01  3.427e-02  -5.927 3.15e-09 ***
wtd_entropy_atomic_mass             5.337e+01  2.139e+00  24.953  < 2e-16 ***
wtd_entropy_atomic_radius          -1.763e+01  3.211e+00  -5.489 4.10e-08 ***
wtd_entropy_FusionHeat              1.353e+01  1.632e+00   8.290  < 2e-16 ***
wtd_entropy_Valence                -2.633e+01  2.404e+00 -10.950  < 2e-16 ***
wtd_gmean_Density                   2.666e-03  1.954e-04  13.643  < 2e-16 ***
wtd_gmean_Valence                   7.947e+00  3.762e+00   2.112  0.03467 *
wtd_mean_Valence                   -2.887e+01  3.322e+00  -8.691  < 2e-16 ***
wtd_std_atomic_radius               3.410e-01  4.597e-02   7.417 1.26e-13 ***
wtd_std_fie                        -1.415e-01  9.531e-03 -14.844  < 2e-16 ***
wtd_std_ThermalConductivity         2.935e-01  1.271e-02  23.084  < 2e-16 ***
entropy_atomic_radius:entropy_fie   1.157e+02  1.205e+01   9.596  < 2e-16 ***
wtd_gmean_Valence:wtd_mean_Valence  2.540e+00  1.926e-01  13.186  < 2e-16 ***
entropy_fie:entropy_Valence        -1.586e+02  1.226e+01 -12.931  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 20.15 on 14855 degrees of freedom
Multiple R-squared:  0.6548,Adjusted R-squared:  0.6541
F-statistic:  1006 on 28 and 14855 DF,  p-value: < 2.2e-16
```

Still the adjusted R square val is significantly low compared to all predictors list. So we can ignore this model

4.1.4 Linear Fit by taking only the relevant columns based on the no of starts that is based on the p value

[41]:
```
fit.starred = lm(critical_temp~.-wtd_entropy_atomic_mass
                 -wtd_range_atomic_mass
                 -wtd_std_atomic_mass
                 -wtd_std_fie
                 -gmean_atomic_radius
                 -wtd_mean_Density
                 -wtd_range_Density
                 -mean_ElectronAffinity
                 -entropy_ElectronAffinity
                 -std_FusionHeat
                 -mean_ThermalConductivity
                 -wtd_entropy_ThermalConductivity
                 -wtd_std_ThermalConductivity
                 -wtd_range_Valence, data = train)
fit.starred.summary = summary(fit.starred)
```

[42]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.starred.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 67 predictors is been used"
```

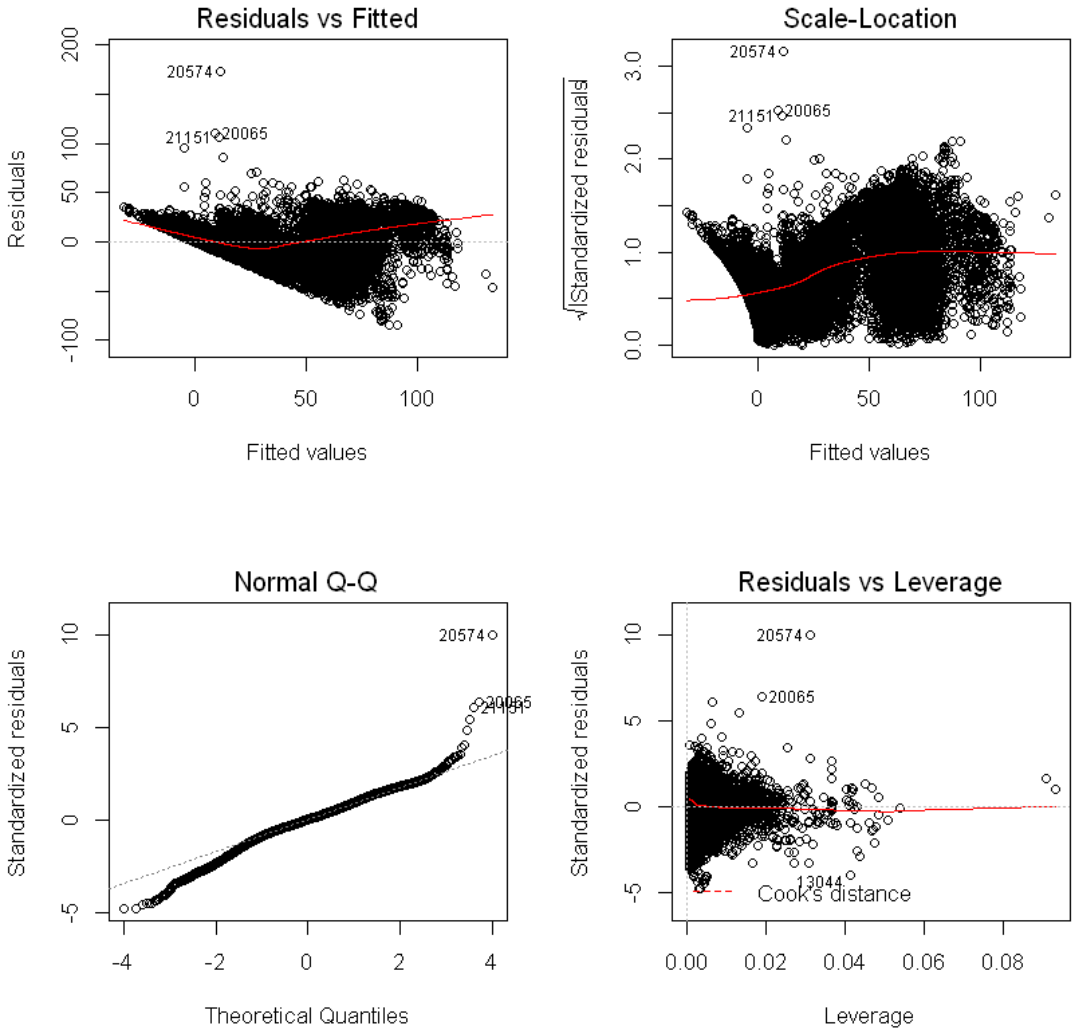
[43]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.all.summary$adj.r.
 ↪squared,4)))
print(paste("Starred Data - Adjusted R-Square:",round(fit.starred.summary$adj.r.
 ↪squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7355"
[1] "Starred Data - Adjusted R-Square: 0.7353"
```

Here we can see that the adjusted R-square is decreased but only for a small amount which indicates that it might be a better model compared to original model(including all predicates) as this model is comparitively less complex

Lets Check the various Residuals plot

[44]:
```
par(mfcol=c(2,2))
plot(fit.starred)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if

residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.5 Perform F-tests by comparing the two models using the anova() function

[45]:
```
anova(fit.all, fit.starred)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14816	4602237	-14	-7338.493	1.688587	0.0507471

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are more correlated as p value is approx 0.05. we can also see that in the new fit the no of predictors is less compared to the original which makes it less complex. Also we can see that there is only slight increase in RSS compared to the original fit. So due to all these factors the new model looks better than the all predictors model

4.1.6 Generating a linear Fit using forward step function

[46]:
```
fit.step.forward = step(lm(critical_temp~1 , data = train),direction =␣
 ↪"forward",scope=formula(lm(critical_temp~.,train)))
fit.step.forward.summary <-summary(fit.step.forward)
fit.step.forward.summary
```

```
Start:  AIC=105198.7
critical_temp ~ 1

                                 Df Sum of Sq      RSS    AIC
+ wtd_std_ThermalConductivity     1   8987862  8478982  94444
+ range_ThermalConductivity       1   8153369  9313475  95841
+ range_atomic_radius             1   7408660 10058184  96986
+ std_ThermalConductivity         1   7343367 10123477  97082
+ wtd_mean_Valence                1   6924525 10542319  97686
```

```
+ wtd_entropy_atomic_mass          1   6846383 10620461  97796
+ wtd_gmean_Valence                1   6562183 10904661  98189
+ wtd_entropy_atomic_radius        1   6354133 11112712  98470
+ number_of_elements               1   6335866 11130978  98494
+ range_fie                        1   6316153 11150692  98521
+ entropy_Valence                  1   6250852 11215992  98608
+ mean_Valence                     1   6190097 11276747  98688
+ wtd_std_atomic_radius            1   6175168 11291676  98708
+ wtd_entropy_Valence              1   6105998 11360846  98799
+ wtd_std_fie                      1   5837654 11629190  99146
+ gmean_Valence                    1   5651312 11815532  99383
+ entropy_fie                      1   5639550 11827294  99398
+ wtd_entropy_FusionHeat           1   5540507 11926337  99522
+ entropy_atomic_radius            1   5469106 11997738  99611
+ std_atomic_radius                1   5390767 12076077  99707
+ entropy_FusionHeat               1   5331323 12135521  99780
+ entropy_atomic_mass              1   5153026 12313818  99998
+ std_fie                          1   5116714 12350130 100041
+ gmean_Density                    1   5113176 12353668 100046
+ wtd_gmean_Density                1   5063413 12403431 100105
+ range_atomic_mass                1   4234379 13232465 101068
+ wtd_range_ThermalConductivity    1   3812287 13654557 101536
+ entropy_Density                  1   3632776 13834068 101730
+ wtd_range_Valence                1   3376931 14089913 102003
+ entropy_ElectronAffinity         1   3299540 14167304 102085
+ wtd_gmean_FusionHeat             1   3251111 14215733 102135
+ wtd_mean_Density                 1   3247803 14219041 102139
+ gmean_FusionHeat                 1   3238689 14228155 102148
+ wtd_entropy_Density              1   2806930 14659914 102593
+ wtd_gmean_atomic_radius          1   2780245 14686599 102620
+ wtd_mean_fie                     1   2721897 14744947 102679
+ wtd_mean_FusionHeat              1   2703449 14763395 102698
+ wtd_entropy_fie                  1   2694345 14772499 102707
+ gmean_ThermalConductivity        1   2604543 14862301 102797
+ gmean_ElectronAffinity           1   2599583 14867261 102802
+ mean_FusionHeat                  1   2590360 14876484 102812
+ std_atomic_mass                  1   2521310 14945534 102880
+ wtd_mean_ThermalConductivity     1   2487799 14979045 102914
+ mean_ThermalConductivity         1   2417131 15049713 102984
+ wtd_gmean_ThermalConductivity    1   2393822 15073023 103007
+ mean_Density                     1   2347256 15119588 103053
+ wtd_gmean_atomic_mass            1   2332737 15134107 103067
+ wtd_std_atomic_mass              1   2261250 15205594 103137
+ wtd_range_atomic_radius          1   2039082 15427762 103353
+ wtd_gmean_fie                    1   2023279 15443565 103368
+ wtd_range_atomic_mass            1   1961954 15504890 103427
+ wtd_std_ElectronAffinity         1   1760601 15706243 103619
+ wtd_range_FusionHeat             1   1725410 15741434 103653
```

```
+ wtd_mean_atomic_mass             1   1648054 15818790 103726
+ wtd_std_Valence                  1   1557296 15909548 103811
+ wtd_range_fie                    1   1532227 15934617 103834
+ wtd_mean_atomic_radius           1   1482649 15984195 103880
+ range_ElectronAffinity           1   1409338 16057506 103949
+ wtd_range_Density                1   1389305 16077539 103967
+ std_ElectronAffinity             1   1234549 16232295 104110
+ range_Density                    1   1189372 16277472 104151
+ wtd_entropy_ElectronAffinity     1    999963 16466881 104323
+ gmean_atomic_mass                1    897694 16569150 104415
+ wtd_std_Density                  1    751732 16715112 104546
+ std_Valence                      1    741371 16725473 104555
+ std_FusionHeat                   1    721755 16745089 104573
+ mean_ElectronAffinity            1    680898 16785946 104609
+ wtd_std_FusionHeat               1    674065 16792779 104615
+ wtd_range_ElectronAffinity       1    573646 16893198 104704
+ gmean_atomic_radius              1    366073 17100771 104885
+ range_FusionHeat                 1    356146 17110698 104894
+ range_Valence                    1    347914 17118930 104901
+ std_Density                      1    238997 17227847 104996
+ wtd_gmean_ElectronAffinity       1    224399 17242445 105008
+ wtd_entropy_ThermalConductivity  1    212547 17254297 105019
+ mean_atomic_mass                 1    207062 17259782 105023
+ wtd_mean_ElectronAffinity        1    202008 17264836 105028
+ mean_fie                         1    191633 17275211 105037
+ mean_atomic_radius               1    183336 17283508 105044
+ entropy_ThermalConductivity      1    143456 17323388 105078
+ gmean_fie                        1      8869 17457975 105193
<none>                                       17466844 105199

Step:  AIC=94443.86
critical_temp ~ wtd_std_ThermalConductivity

                                 Df Sum of Sq     RSS   AIC
+ gmean_ElectronAffinity          1    688536 7790446 93185
+ wtd_gmean_ElectronAffinity      1    688449 7790533 93185
+ wtd_entropy_atomic_mass         1    606107 7872875 93342
+ range_atomic_radius             1    577016 7901965 93397
+ number_of_elements              1    480358 7998624 93578
+ wtd_entropy_atomic_radius       1    446388 8032594 93641
+ range_fie                       1    432119 8046863 93667
+ wtd_entropy_Valence             1    401215 8077767 93724
+ wtd_mean_Valence                1    396359 8082623 93733
+ mean_Valence                    1    384247 8094735 93756
+ range_atomic_mass               1    377625 8101357 93768
+ entropy_ThermalConductivity     1    364222 8114760 93792
+ wtd_gmean_Valence               1    355078 8123903 93809
+ mean_ElectronAffinity           1    351696 8127286 93815
```

```
+ entropy_Valence                   1    343624 8135358 93830
+ gmean_Valence                     1    341336 8137646 93834
+ wtd_entropy_FusionHeat            1    324955 8154027 93864
+ gmean_Density                     1    316942 8162040 93879
+ wtd_entropy_ThermalConductivity   1    315026 8163956 93882
+ entropy_fie                       1    306193 8172789 93898
+ entropy_atomic_radius             1    278508 8200474 93949
+ std_atomic_radius                 1    267928 8211054 93968
+ wtd_mean_ElectronAffinity         1    261724 8217258 93979
+ std_ThermalConductivity           1    260670 8218312 93981
+ wtd_entropy_fie                   1    258136 8220846 93986
+ wtd_std_atomic_radius             1    245712 8233270 94008
+ std_fie                           1    234290 8244692 94029
+ entropy_FusionHeat                1    222944 8256038 94049
+ std_atomic_mass                   1    222561 8256420 94050
+ wtd_gmean_Density                 1    219099 8259883 94056
+ mean_Density                      1    190550 8288432 94108
+ wtd_entropy_Density               1    179380 8299602 94128
+ entropy_atomic_mass               1    177769 8301213 94130
+ wtd_range_atomic_mass             1    162661 8316321 94158
+ wtd_std_fie                       1    161567 8317415 94160
+ wtd_mean_Density                  1    156559 8322423 94168
+ wtd_range_Valence                 1    125989 8352992 94223
+ gmean_ThermalConductivity         1    124676 8354306 94225
+ mean_ThermalConductivity          1    116747 8362235 94239
+ wtd_range_atomic_radius           1    100474 8378507 94268
+ entropy_Density                   1     97353 8381629 94274
+ wtd_std_Valence                   1     89260 8389722 94288
+ wtd_gmean_ThermalConductivity     1     88907 8390075 94289
+ wtd_range_ElectronAffinity        1     79245 8399737 94306
+ wtd_gmean_atomic_mass             1     74952 8404030 94314
+ wtd_mean_atomic_mass              1     71144 8407838 94320
+ gmean_atomic_mass                 1     70247 8408734 94322
+ gmean_FusionHeat                  1     69906 8409076 94323
+ wtd_std_ElectronAffinity          1     69096 8409885 94324
+ wtd_range_Density                 1     66501 8412481 94329
+ range_ElectronAffinity            1     63656 8415326 94334
+ std_ElectronAffinity              1     59898 8419084 94340
+ mean_fie                          1     54854 8424128 94349
+ mean_FusionHeat                   1     35900 8443081 94383
+ wtd_std_atomic_mass               1     33202 8445779 94387
+ std_Valence                       1     28172 8450810 94396
+ wtd_std_FusionHeat                1     23799 8455183 94404
+ gmean_fie                         1     22258 8456724 94407
+ wtd_mean_fie                      1     20837 8458145 94409
+ wtd_gmean_FusionHeat              1     20582 8458399 94410
+ wtd_std_Density                   1     20501 8458481 94410
+ range_ThermalConductivity         1     18981 8460001 94412
```

```
+ mean_atomic_mass                1     17932 8461050 94414
+ gmean_atomic_radius             1     17399 8461583 94415
+ wtd_range_ThermalConductivity   1     15851 8463131 94418
+ wtd_mean_FusionHeat             1     14971 8464010 94420
+ range_Density                   1     14280 8464702 94421
+ wtd_gmean_atomic_radius         1     12371 8466611 94424
+ wtd_gmean_fie                   1     10077 8468905 94428
+ entropy_ElectronAffinity        1      7837 8471145 94432
+ wtd_range_FusionHeat            1      5357 8473624 94436
+ std_FusionHeat                  1      5335 8473646 94436
+ wtd_range_fie                   1      3194 8475787 94440
+ range_FusionHeat                1      1327 8477655 94444
+ mean_atomic_radius              1      1308 8477674 94444
<none>                                       8478982 94444
+ wtd_entropy_ElectronAffinity    1       833 8478149 94444
+ range_Valence                   1       746 8478236 94445
+ std_Density                     1       185 8478797 94446
+ wtd_mean_ThermalConductivity    1       184 8478798 94446
+ wtd_mean_atomic_radius          1         1 8478981 94446

Step:  AIC=93185.3
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity

                                Df Sum of Sq     RSS   AIC
+ range_atomic_radius            1    423805 7366641 92355
+ wtd_entropy_atomic_mass        1    384408 7406038 92434
+ range_fie                      1    364652 7425794 92474
+ range_atomic_mass              1    307636 7482810 92588
+ wtd_entropy_Valence            1    265736 7524710 92671
+ wtd_entropy_atomic_radius      1    264053 7526393 92674
+ number_of_elements            1    248076 7542370 92706
+ std_atomic_radius              1    231309 7559137 92739
+ std_fie                        1    223593 7566853 92754
+ std_atomic_mass                1    215233 7575213 92770
+ mean_fie                       1    207363 7583083 92786
+ wtd_entropy_fie                1    199962 7590484 92800
+ wtd_entropy_FusionHeat         1    186158 7604288 92827
+ std_ThermalConductivity        1    185789 7604657 92828
+ wtd_std_atomic_radius          1    183367 7607079 92833
+ entropy_Valence                1    158666 7631780 92881
+ gmean_Density                  1    157108 7633338 92884
+ gmean_fie                      1    154078 7636368 92890
+ entropy_fie                    1    137829 7652617 92922
+ wtd_entropy_ThermalConductivity 1   133205 7657241 92931
+ wtd_std_ElectronAffinity       1    120994 7669452 92954
+ std_ElectronAffinity           1    120141 7670305 92956
+ gmean_ThermalConductivity      1    119298 7671148 92958
+ range_ElectronAffinity         1    115756 7674690 92964
```

```
+ wtd_std_fie                       1    115688 7674758 92965
+ entropy_atomic_radius             1    112765 7677681 92970
+ entropy_ThermalConductivity       1    108765 7681681 92978
+ wtd_entropy_Density               1    102743 7687703 92990
+ mean_ElectronAffinity             1    101018 7689428 92993
+ wtd_range_atomic_mass             1     99535 7690911 92996
+ wtd_gmean_Density                 1     96433 7694013 93002
+ wtd_range_atomic_radius           1     93174 7697272 93008
+ mean_ThermalConductivity          1     90753 7699693 93013
+ wtd_gmean_ElectronAffinity        1     88246 7702200 93018
+ mean_Valence                      1     75930 7714517 93042
+ wtd_mean_Valence                  1     75338 7715108 93043
+ gmean_atomic_radius               1     72802 7717644 93048
+ wtd_gmean_ThermalConductivity     1     71178 7719268 93051
+ mean_Density                      1     68677 7721769 93056
+ gmean_Valence                     1     68053 7722393 93057
+ entropy_FusionHeat                1     66040 7724406 93061
+ wtd_std_Valence                   1     64365 7726081 93064
+ wtd_gmean_Valence                 1     62581 7727865 93067
+ wtd_range_Valence                 1     61583 7728863 93069
+ entropy_atomic_mass               1     58072 7732374 93076
+ wtd_mean_Density                  1     49258 7741188 93093
+ range_ThermalConductivity         1     46289 7744157 93099
+ wtd_std_atomic_mass               1     44464 7745982 93102
+ wtd_mean_fie                      1     42204 7748242 93106
+ wtd_gmean_fie                     1     34257 7756189 93122
+ wtd_range_Density                 1     33256 7757190 93124
+ entropy_ElectronAffinity          1     30001 7760445 93130
+ gmean_FusionHeat                  1     26790 7763656 93136
+ wtd_entropy_ElectronAffinity      1     26128 7764318 93137
+ range_Density                     1     25253 7765193 93139
+ entropy_Density                   1     17858 7772588 93153
+ std_Valence                       1     15622 7774824 93157
+ wtd_range_fie                     1     15233 7775213 93158
+ gmean_atomic_mass                 1     14691 7775755 93159
+ wtd_std_FusionHeat                1     14151 7776295 93160
+ wtd_gmean_atomic_mass             1     14045 7776401 93160
+ mean_atomic_radius                1     13815 7776631 93161
+ wtd_gmean_atomic_radius           1     12794 7777652 93163
+ wtd_mean_atomic_mass              1      9571 7780875 93169
+ mean_FusionHeat                   1      9110 7781336 93170
+ std_Density                       1      9035 7781411 93170
+ wtd_range_ElectronAffinity        1      7762 7782684 93172
+ wtd_mean_ElectronAffinity         1      6304 7784142 93175
+ wtd_range_ThermalConductivity     1      3479 7786967 93181
+ wtd_range_FusionHeat              1      3406 7787040 93181
+ wtd_gmean_FusionHeat              1      3272 7787174 93181
+ wtd_mean_ThermalConductivity      1      2163 7788283 93183
```

```
+ std_FusionHeat                   1      2044 7788402 93183
+ wtd_mean_FusionHeat              1      1839 7788607 93184
<none>                                       7790446 93185
+ range_FusionHeat                1       861 7789585 93186
+ wtd_std_Density                  1       680 7789766 93186
+ wtd_mean_atomic_radius           1       490 7789956 93186
+ mean_atomic_mass                 1       127 7790319 93187
+ range_Valence                    1        27 7790419 93187

Step:  AIC=92354.74
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius

                                  Df Sum of Sq     RSS   AIC
+ std_atomic_radius                1    240565 7126076 91863
+ wtd_gmean_ElectronAffinity       1    203297 7163345 91940
+ std_ThermalConductivity          1    178698 7187943 91991
+ wtd_std_Valence                  1    172959 7193683 92003
+ wtd_std_atomic_radius            1    159730 7206912 92030
+ wtd_mean_atomic_radius           1    107009 7259633 92139
+ wtd_entropy_atomic_mass          1    105543 7261099 92142
+ wtd_std_FusionHeat               1    105077 7261564 92143
+ wtd_gmean_atomic_radius          1    102722 7263919 92148
+ wtd_range_fie                    1    101180 7265462 92151
+ range_ThermalConductivity        1     94368 7272273 92165
+ std_Valence                      1     88624 7278018 92177
+ wtd_range_ElectronAffinity       1     79019 7287623 92196
+ range_atomic_mass                1     74347 7292295 92206
+ wtd_mean_ThermalConductivity     1     73194 7293448 92208
+ wtd_gmean_atomic_mass            1     67080 7299562 92221
+ wtd_entropy_ThermalConductivity  1     61325 7305317 92232
+ gmean_fie                        1     56502 7310139 92242
+ wtd_std_fie                      1     56485 7310157 92242
+ range_FusionHeat                 1     55330 7311312 92245
+ std_FusionHeat                   1     53838 7312803 92248
+ range_Valence                    1     50385 7316257 92255
+ wtd_entropy_fie                  1     49043 7317599 92257
+ mean_fie                         1     47945 7318696 92260
+ wtd_entropy_FusionHeat           1     44825 7321817 92266
+ std_atomic_mass                  1     44706 7321935 92266
+ entropy_ElectronAffinity         1     42668 7323973 92270
+ wtd_entropy_Valence              1     38297 7328344 92279
+ wtd_std_Density                  1     37987 7328655 92280
+ entropy_ThermalConductivity      1     37533 7329109 92281
+ wtd_mean_fie                     1     35903 7330739 92284
+ mean_atomic_mass                 1     34040 7332601 92288
+ number_of_elements               1     31835 7334806 92292
+ wtd_mean_atomic_mass             1     31332 7335309 92293
```

```
+ wtd_gmean_fie                   1     29855 7336787 92296
+ gmean_atomic_mass               1     28002 7338640 92300
+ mean_ElectronAffinity           1     27873 7338769 92300
+ wtd_gmean_Density               1     26136 7340505 92304
+ wtd_mean_ElectronAffinity       1     23768 7342874 92309
+ wtd_range_atomic_mass           1     21814 7344827 92313
+ wtd_entropy_atomic_radius       1     20102 7346540 92316
+ wtd_entropy_Density             1     17376 7349266 92322
+ wtd_mean_Density                1     16325 7350316 92324
+ range_fie                       1     13848 7352793 92329
+ std_ElectronAffinity           1     13049 7353592 92330
+ gmean_Valence                  1     12992 7353649 92330
+ wtd_std_ElectronAffinity       1     11855 7354787 92333
+ wtd_std_atomic_mass            1     11798 7354844 92333
+ wtd_range_FusionHeat           1     11251 7355390 92334
+ wtd_range_atomic_radius        1      9627 7357015 92337
+ wtd_range_Valence              1      9464 7357178 92338
+ wtd_range_ThermalConductivity  1      6819 7359822 92343
+ std_fie                        1      6818 7359824 92343
+ wtd_entropy_ElectronAffinity   1      6721 7359921 92343
+ wtd_gmean_Valence              1      5493 7361148 92346
+ entropy_FusionHeat             1      5373 7361269 92346
+ mean_Valence                   1      4779 7361862 92347
+ range_ElectronAffinity         1      4674 7361967 92347
+ entropy_Density                1      4004 7362638 92349
+ gmean_Density                  1      3685 7362957 92349
+ gmean_ThermalConductivity      1      3266 7363375 92350
+ mean_Density                   1      3193 7363448 92350
+ mean_ThermalConductivity       1      2592 7364050 92352
+ mean_FusionHeat                1      2517 7364124 92352
+ entropy_atomic_mass            1      1676 7364966 92353
+ wtd_mean_FusionHeat            1      1596 7365045 92354
+ entropy_Valence                1       996 7365645 92355
<none>                                      7366641 92355
+ wtd_gmean_FusionHeat           1       925 7365716 92355
+ wtd_gmean_ThermalConductivity  1       624 7366018 92355
+ wtd_mean_Valence               1       602 7366040 92356
+ gmean_FusionHeat               1       221 7366420 92356
+ mean_atomic_radius             1       210 7366432 92356
+ std_Density                    1       164 7366477 92356
+ entropy_fie                    1        82 7366559 92357
+ entropy_atomic_radius          1        62 7366579 92357
+ range_Density                  1        37 7366604 92357
+ gmean_atomic_radius            1        22 7366620 92357
+ wtd_range_Density              1         1 7366641 92357

Step:  AIC=91862.58
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
```

```
    range_atomic_radius + std_atomic_radius

                                  Df Sum of Sq     RSS   AIC
+ entropy_ElectronAffinity         1    277891 6848186 91273
+ wtd_std_Valence                  1    194160 6931916 91453
+ entropy_atomic_mass              1    186058 6940018 91471
+ wtd_gmean_ElectronAffinity       1    184386 6941690 91474
+ range_ThermalConductivity        1    183760 6942317 91476
+ entropy_Density                  1    182503 6943573 91478
+ std_ThermalConductivity          1    143351 6982725 91562
+ entropy_atomic_radius            1    137930 6988146 91574
+ entropy_fie                      1    121366 7004710 91609
+ entropy_Valence                  1    106757 7019319 91640
+ std_Valence                      1    103116 7022960 91648
+ wtd_mean_ThermalConductivity     1    102909 7023168 91648
+ entropy_FusionHeat               1     98794 7027282 91657
+ range_Valence                    1     83092 7042984 91690
+ wtd_std_atomic_radius            1     77100 7048976 91703
+ wtd_range_fie                    1     75716 7050361 91706
+ wtd_mean_atomic_radius           1     73555 7052522 91710
+ wtd_std_fie                      1     72019 7054057 91713
+ wtd_gmean_atomic_radius          1     70091 7055985 91717
+ gmean_fie                        1     62040 7064036 91734
+ mean_fie                         1     61409 7064667 91736
+ wtd_entropy_ElectronAffinity     1     58205 7067871 91743
+ wtd_range_ElectronAffinity       1     56136 7069940 91747
+ number_of_elements               1     53197 7072880 91753
+ wtd_std_Density                  1     44811 7081265 91771
+ wtd_std_FusionHeat               1     35760 7090317 91790
+ wtd_std_atomic_mass              1     34294 7091782 91793
+ wtd_mean_ElectronAffinity        1     30926 7095151 91800
+ wtd_range_ThermalConductivity    1     30606 7095470 91801
+ wtd_range_atomic_mass            1     29899 7096178 91802
+ wtd_mean_fie                     1     27336 7098740 91807
+ wtd_gmean_FusionHeat             1     22115 7103961 91818
+ std_atomic_mass                  1     21106 7104970 91820
+ wtd_gmean_fie                    1     20462 7105614 91822
+ wtd_entropy_Density              1     19856 7106220 91823
+ wtd_gmean_atomic_mass            1     19821 7106256 91823
+ mean_ElectronAffinity            1     19571 7106505 91824
+ range_atomic_mass                1     19488 7106588 91824
+ range_FusionHeat                 1     14405 7111671 91834
+ wtd_gmean_Density                1     13461 7112616 91836
+ std_ElectronAffinity             1     10816 7115261 91842
+ wtd_entropy_atomic_mass          1     10163 7115913 91843
+ wtd_entropy_atomic_radius        1      9976 7116100 91844
+ wtd_mean_FusionHeat              1      9949 7116127 91844
+ wtd_range_atomic_radius          1      7772 7118304 91848
```

```
+ gmean_atomic_radius               1      7143 7118933 91850
+ wtd_entropy_ThermalConductivity   1      6883 7119194 91850
+ range_Density                     1      6452 7119625 91851
+ std_FusionHeat                    1      6365 7119711 91851
+ gmean_FusionHeat                  1      5229 7120848 91854
+ wtd_std_ElectronAffinity          1      5167 7120910 91854
+ wtd_range_FusionHeat              1      4763 7121314 91855
+ mean_Density                      1      4345 7121731 91855
+ mean_FusionHeat                   1      4202 7121874 91856
+ wtd_gmean_Valence                 1      4197 7121879 91856
+ wtd_entropy_FusionHeat            1      4143 7121933 91856
+ wtd_entropy_fie                   1      4135 7121941 91856
+ wtd_range_Valence                 1      3602 7122475 91857
+ wtd_mean_Density                  1      3419 7122657 91857
+ entropy_ThermalConductivity       1      3030 7123046 91858
+ wtd_mean_atomic_mass              1      2742 7123334 91859
+ gmean_Valence                     1      2500 7123577 91859
+ mean_atomic_radius                1      2346 7123730 91860
+ mean_atomic_mass                  1      1828 7124248 91861
+ std_Density                       1      1679 7124397 91861
+ wtd_entropy_Valence               1      1379 7124697 91862
+ wtd_gmean_ThermalConductivity     1      1272 7124804 91862
+ range_fie                         1       959 7125117 91863
<none>                                       7126076 91863
+ wtd_range_Density                 1       688 7125388 91863
+ gmean_Density                     1       551 7125525 91863
+ std_fie                           1       248 7125828 91864
+ range_ElectronAffinity            1       229 7125847 91864
+ gmean_atomic_mass                 1       213 7125864 91864
+ gmean_ThermalConductivity         1       199 7125878 91864
+ wtd_mean_Valence                  1       163 7125913 91864
+ mean_ThermalConductivity          1        78 7125998 91864
+ mean_Valence                      1         2 7126074 91865

Step:  AIC=91272.53
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity

                                Df Sum of Sq     RSS   AIC
+ wtd_gmean_ElectronAffinity     1    237435 6610751 90749
+ wtd_entropy_atomic_mass        1    150622 6697564 90944
+ std_ThermalConductivity        1    141198 6706988 90964
+ wtd_entropy_ThermalConductivity 1   139822 6708363 90967
+ range_ThermalConductivity      1    130631 6717555 90988
+ wtd_entropy_fie                 1    110110 6738076 91033
+ wtd_gmean_atomic_radius         1     96900 6751285 91062
+ entropy_ThermalConductivity     1     96326 6751859 91064
+ wtd_mean_atomic_radius          1     92781 6755405 91072
```

```
+ wtd_std_Valence                  1     88092 6760094 91082
+ wtd_std_atomic_radius            1     85683 6762503 91087
+ wtd_entropy_Valence              1     81773 6766412 91096
+ wtd_std_fie                      1     81519 6766667 91096
+ wtd_mean_ElectronAffinity        1     80914 6767271 91098
+ wtd_range_ElectronAffinity       1     80500 6767685 91099
+ wtd_mean_ThermalConductivity     1     78765 6769421 91102
+ wtd_range_fie                    1     69679 6778506 91122
+ wtd_mean_fie                     1     69667 6778519 91122
+ wtd_gmean_fie                    1     58935 6789251 91146
+ range_atomic_mass                1     56975 6791211 91150
+ wtd_entropy_FusionHeat           1     55679 6792506 91153
+ number_of_elements               1     55243 6792942 91154
+ wtd_entropy_atomic_radius        1     52469 6795717 91160
+ std_atomic_mass                  1     43123 6805063 91181
+ entropy_Valence                  1     34968 6813218 91198
+ wtd_std_Density                  1     33035 6815150 91203
+ std_Valence                      1     32450 6815735 91204
+ entropy_fie                      1     28780 6819405 91212
+ wtd_range_ThermalConductivity    1     20098 6828088 91231
+ gmean_fie                        1     19535 6828651 91232
+ mean_fie                         1     18613 6829573 91234
+ entropy_atomic_radius            1     18290 6829896 91235
+ wtd_entropy_Density              1     18136 6830050 91235
+ wtd_std_atomic_mass              1     17226 6830960 91237
+ wtd_std_FusionHeat               1     14350 6833835 91243
+ wtd_gmean_FusionHeat             1     14340 6833846 91243
+ wtd_gmean_atomic_mass            1     13403 6834783 91245
+ range_Valence                    1     12454 6835731 91247
+ wtd_gmean_Density                1     11086 6837099 91250
+ wtd_range_atomic_mass            1     11080 6837105 91250
+ wtd_entropy_ElectronAffinity     1      9873 6838313 91253
+ entropy_FusionHeat               1      9336 6838850 91254
+ mean_Density                     1      7651 6840535 91258
+ wtd_mean_FusionHeat              1      6148 6842038 91261
+ mean_ThermalConductivity         1      5166 6843020 91263
+ wtd_range_FusionHeat             1      5050 6843136 91264
+ wtd_range_Density                1      4682 6843504 91264
+ range_fie                        1      4319 6843867 91265
+ entropy_Density                  1      2768 6845417 91269
+ wtd_mean_Density                 1      2533 6845653 91269
+ gmean_atomic_radius              1      2096 6846090 91270
+ mean_FusionHeat                  1      1789 6846397 91271
+ entropy_atomic_mass              1      1593 6846592 91271
+ wtd_gmean_Valence                1      1570 6846616 91271
+ gmean_FusionHeat                 1      1550 6846636 91271
+ gmean_ThermalConductivity        1      1355 6846830 91272
+ wtd_mean_atomic_mass             1      1353 6846832 91272
```

```
+ range_Density                    1      1353 6846833 91272
+ gmean_Density                    1      1119 6847067 91272
+ std_ElectronAffinity             1      1090 6847096 91272
+ gmean_Valence                    1       946 6847240 91272
<none>                                       6848186 91273
+ mean_ElectronAffinity            1       864 6847321 91273
+ mean_atomic_radius               1       757 6847428 91273
+ range_FusionHeat                 1       605 6847581 91273
+ mean_atomic_mass                 1       602 6847584 91273
+ std_fie                          1       548 6847637 91273
+ std_Density                      1       532 6847654 91273
+ wtd_range_Valence                1       453 6847732 91274
+ gmean_atomic_mass                1       267 6847919 91274
+ std_FusionHeat                   1       264 6847922 91274
+ wtd_gmean_ThermalConductivity    1       217 6847969 91274
+ wtd_std_ElectronAffinity         1       163 6848023 91274
+ range_ElectronAffinity           1        70 6848116 91274
+ wtd_range_atomic_radius          1        53 6848133 91274
+ wtd_mean_Valence                 1        26 6848160 91274
+ mean_Valence                     1         5 6848180 91275

Step:  AIC=90749.33
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity

                                  Df Sum of Sq     RSS   AIC
+ wtd_std_Valence                  1    155729 6455022 90397
+ wtd_entropy_atomic_mass          1    121619 6489132 90475
+ entropy_ThermalConductivity      1     94894 6515857 90536
+ std_ThermalConductivity          1     90112 6520639 90547
+ range_ThermalConductivity        1     70009 6540742 90593
+ wtd_entropy_ThermalConductivity  1     55245 6555506 90626
+ std_Valence                      1     54498 6556253 90628
+ wtd_entropy_ElectronAffinity     1     46957 6563794 90645
+ wtd_mean_ElectronAffinity        1     45557 6565194 90648
+ range_atomic_mass                1     44884 6565867 90650
+ wtd_mean_ThermalConductivity     1     43629 6567122 90653
+ wtd_entropy_atomic_radius        1     43142 6567609 90654
+ number_of_elements               1     42680 6568071 90655
+ wtd_std_atomic_radius            1     40370 6570381 90660
+ entropy_Valence                  1     38106 6572645 90665
+ range_Valence                    1     32716 6578036 90677
+ std_atomic_mass                  1     31708 6579043 90680
+ wtd_range_Valence                1     30520 6580231 90682
+ wtd_std_fie                      1     29366 6581385 90685
+ wtd_std_Density                  1     27084 6583667 90690
+ wtd_entropy_FusionHeat           1     23354 6587397 90699
```

```
+ entropy_fie                      1     23086 6587665 90699
+ wtd_std_FusionHeat               1     19679 6591072 90707
+ entropy_atomic_radius            1     18991 6591760 90709
+ wtd_std_atomic_mass              1     18731 6592020 90709
+ wtd_range_ThermalConductivity    1     17987 6592764 90711
+ wtd_range_ElectronAffinity       1     15026 6595725 90717
+ entropy_FusionHeat               1     13133 6597618 90722
+ wtd_range_FusionHeat             1     13062 6597689 90722
+ wtd_gmean_atomic_radius          1     11753 6598998 90725
+ wtd_gmean_FusionHeat             1     11552 6599199 90725
+ wtd_gmean_Valence                1     11439 6599312 90726
+ wtd_mean_atomic_radius           1     10919 6599832 90727
+ wtd_range_Density                1     10522 6600229 90728
+ wtd_gmean_Density                1     10214 6600537 90728
+ wtd_gmean_atomic_mass            1      8529 6602222 90732
+ wtd_entropy_Valence              1      7984 6602767 90733
+ mean_atomic_mass                 1      6164 6604587 90737
+ wtd_range_atomic_mass            1      5652 6605099 90739
+ mean_Density                     1      5222 6605529 90740
+ wtd_mean_FusionHeat              1      4583 6606168 90741
+ wtd_entropy_fie                  1      4555 6606196 90741
+ wtd_mean_Valence                 1      3352 6607399 90744
+ gmean_atomic_mass                1      3235 6607516 90744
+ range_FusionHeat                 1      3063 6607688 90744
+ mean_atomic_radius               1      2993 6607758 90745
+ wtd_std_ElectronAffinity         1      2900 6607851 90745
+ range_Density                    1      2819 6607933 90745
+ wtd_range_fie                    1      2383 6608368 90746
+ range_fie                        1      2111 6608640 90747
+ std_Density                      1      2025 6608726 90747
+ std_FusionHeat                   1      1528 6609223 90748
+ wtd_range_atomic_radius          1      1419 6609332 90748
+ mean_fie                         1      1162 6609589 90749
+ gmean_ThermalConductivity        1      1114 6609637 90749
+ range_ElectronAffinity           1       981 6609770 90749
+ gmean_fie                        1       953 6609798 90749
+ gmean_atomic_radius              1       926 6609825 90749
+ mean_ThermalConductivity         1       924 6609827 90749
<none>                                       6610751 90749
+ gmean_Valence                    1       648 6610103 90750
+ std_fie                          1       627 6610124 90750
+ wtd_mean_fie                     1       451 6610300 90750
+ wtd_mean_Density                 1       312 6610439 90751
+ mean_ElectronAffinity            1       278 6610473 90751
+ mean_Valence                     1       216 6610535 90751
+ entropy_Density                  1       197 6610554 90751
+ wtd_mean_atomic_mass             1       168 6610583 90751
+ wtd_entropy_Density              1       107 6610644 90751
```

```
+ mean_FusionHeat                   1        63 6610688 90751
+ wtd_gmean_ThermalConductivity     1        34 6610717 90751
+ wtd_gmean_fie                     1        23 6610728 90751
+ std_ElectronAffinity              1        17 6610734 90751
+ entropy_atomic_mass               1         5 6610746 90751
+ gmean_FusionHeat                  1         0 6610751 90751
+ gmean_Density                     1         0 6610751 90751

Step:  AIC=90396.51
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence

                                Df Sum of Sq     RSS   AIC
+ wtd_entropy_atomic_mass        1    157739 6297283 90030
+ wtd_mean_ElectronAffinity      1    156477 6298545 90033
+ wtd_entropy_atomic_radius      1    137015 6318007 90079
+ entropy_ThermalConductivity    1    122725 6332297 90113
+ wtd_entropy_ThermalConductivity 1    119526 6335496 90120
+ number_of_elements             1     94286 6360736 90180
+ range_atomic_mass              1     90556 6364466 90188
+ entropy_fie                    1     80846 6374176 90211
+ range_Valence                  1     80587 6374435 90212
+ std_ThermalConductivity        1     80117 6374905 90213
+ entropy_atomic_radius          1     76388 6378634 90221
+ std_atomic_mass                1     62964 6392058 90253
+ wtd_entropy_fie                1     60504 6394518 90258
+ range_ThermalConductivity      1     58678 6396344 90263
+ wtd_entropy_FusionHeat         1     57541 6397481 90265
+ wtd_mean_ThermalConductivity   1     50733 6404289 90281
+ std_Valence                    1     43650 6411372 90298
+ wtd_std_atomic_radius          1     42726 6412296 90300
+ entropy_Valence                1     40429 6414593 90305
+ wtd_range_ElectronAffinity     1     40151 6414871 90306
+ wtd_range_Valence              1     34308 6420714 90319
+ wtd_entropy_Valence            1     34115 6420907 90320
+ mean_ElectronAffinity          1     30195 6424827 90329
+ entropy_FusionHeat             1     23292 6431730 90345
+ std_ElectronAffinity           1     22013 6433009 90348
+ wtd_std_fie                    1     19271 6435751 90354
+ wtd_range_atomic_radius        1     17884 6437138 90357
+ wtd_range_ThermalConductivity  1     17644 6437378 90358
+ wtd_entropy_ElectronAffinity   1     17109 6437913 90359
+ wtd_std_FusionHeat             1     16971 6438051 90359
+ wtd_mean_Valence               1     16010 6439012 90362
+ wtd_std_ElectronAffinity       1     14303 6440719 90365
+ wtd_gmean_Valence              1     13032 6441990 90368
+ range_fie                      1     12471 6442551 90370
```

```
+ range_ElectronAffinity           1     11059 6443963 90373
+ wtd_range_Density                1     10686 6444335 90374
+ mean_fie                         1      9498 6445524 90377
+ mean_Density                     1      9447 6445575 90377
+ gmean_fie                        1      8747 6446275 90378
+ wtd_range_FusionHeat             1      8264 6446758 90379
+ wtd_gmean_atomic_radius          1      7373 6447649 90382
+ wtd_gmean_atomic_mass            1      6613 6448409 90383
+ wtd_entropy_Density              1      5928 6449094 90385
+ wtd_gmean_Density                1      5021 6450001 90387
+ wtd_range_atomic_mass            1      4688 6450334 90388
+ wtd_gmean_FusionHeat             1      4584 6450438 90388
+ wtd_mean_atomic_radius           1      4514 6450508 90388
+ gmean_Density                    1      4065 6450957 90389
+ wtd_std_Density                  1      4032 6450990 90389
+ range_FusionHeat                 1      3644 6451378 90390
+ gmean_FusionHeat                 1      3351 6451670 90391
+ entropy_atomic_mass              1      2721 6452301 90392
+ mean_atomic_mass                 1      2647 6452375 90392
+ std_Density                      1      2479 6452543 90393
+ gmean_atomic_radius              1      2378 6452644 90393
+ gmean_ThermalConductivity        1      2353 6452669 90393
+ std_FusionHeat                   1      1895 6453127 90394
+ wtd_range_fie                    1      1844 6453178 90394
+ mean_FusionHeat                  1      1606 6453416 90395
+ range_Density                    1      1506 6453516 90395
+ wtd_mean_FusionHeat              1      1399 6453623 90395
+ std_fie                          1      1394 6453628 90395
+ mean_atomic_radius               1      1266 6453756 90396
+ wtd_std_atomic_mass              1      1113 6453909 90396
<none>                                       6455022 90397
+ entropy_Density                 1       866 6454156 90397
+ wtd_mean_atomic_mass            1       866 6454156 90397
+ wtd_gmean_fie                   1       847 6454175 90397
+ wtd_mean_Density                1       706 6454315 90397
+ mean_Valence                    1       226 6454796 90398
+ gmean_Valence                   1       186 6454836 90398
+ wtd_gmean_ThermalConductivity   1       159 6454863 90398
+ gmean_atomic_mass               1        54 6454968 90398
+ wtd_mean_fie                    1        17 6455005 90398
+ mean_ThermalConductivity        1        13 6455009 90398

Step:  AIC=90030.28
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass

                                Df Sum of Sq     RSS   AIC
```

```
+ wtd_entropy_Density               1    103459 6193824 89786
+ wtd_range_Valence                 1     99209 6198074 89796
+ range_atomic_mass                 1     87959 6209324 89823
+ wtd_std_atomic_radius             1     82207 6215076 89837
+ wtd_range_Density                 1     79074 6218209 89844
+ entropy_ThermalConductivity       1     75573 6221709 89853
+ range_Valence                     1     66760 6230523 89874
+ wtd_mean_ThermalConductivity      1     66265 6231018 89875
+ std_atomic_mass                   1     64680 6232603 89879
+ wtd_mean_ElectronAffinity         1     63475 6233808 89881
+ wtd_entropy_ThermalConductivity   1     51026 6246257 89911
+ std_ThermalConductivity           1     50255 6247028 89913
+ std_Valence                       1     41454 6255829 89934
+ wtd_entropy_ElectronAffinity      1     41247 6256036 89934
+ range_ThermalConductivity         1     39621 6257662 89938
+ wtd_std_fie                       1     38109 6259174 89942
+ wtd_range_atomic_mass             1     38038 6259245 89942
+ wtd_range_ThermalConductivity     1     36794 6260489 89945
+ entropy_Density                   1     36336 6260947 89946
+ number_of_elements                1     35051 6262232 89949
+ entropy_atomic_mass               1     30226 6267057 89961
+ wtd_gmean_atomic_radius           1     28848 6268435 89964
+ wtd_std_FusionHeat                1     24398 6272884 89975
+ wtd_range_ElectronAffinity        1     24061 6273222 89975
+ wtd_mean_atomic_radius            1     23571 6273712 89976
+ wtd_range_FusionHeat              1     15281 6282002 89996
+ entropy_fie                       1     15233 6282050 89996
+ wtd_gmean_atomic_mass             1     13683 6283600 90000
+ mean_Density                      1     13100 6284183 90001
+ wtd_mean_Valence                  1     12565 6284718 90003
+ wtd_range_atomic_radius           1     12170 6285113 90003
+ gmean_Density                     1     11535 6285748 90005
+ wtd_entropy_Valence               1     11329 6285954 90005
+ wtd_entropy_fie                   1     10414 6286869 90008
+ entropy_atomic_radius             1     10321 6286962 90008
+ wtd_gmean_Valence                 1      9340 6287943 90010
+ wtd_mean_atomic_mass              1      8994 6288289 90011
+ wtd_gmean_Density                 1      8847 6288436 90011
+ range_fie                         1      8321 6288962 90013
+ wtd_gmean_FusionHeat              1      8250 6289033 90013
+ wtd_mean_fie                      1      8169 6289114 90013
+ wtd_mean_Density                  1      7103 6290180 90015
+ mean_fie                          1      6630 6290653 90017
+ gmean_atomic_radius               1      6126 6291157 90018
+ gmean_fie                         1      5577 6291706 90019
+ mean_ElectronAffinity             1      5515 6291768 90019
+ wtd_std_Density                   1      5440 6291843 90019
+ gmean_Valence                     1      4983 6292300 90020
```

```
+ range_FusionHeat                 1      4491 6292792 90022
+ wtd_entropy_atomic_radius        1      4092 6293191 90023
+ wtd_gmean_fie                    1      3657 6293626 90024
+ mean_atomic_radius               1      3608 6293675 90024
+ wtd_gmean_ThermalConductivity    1      2879 6294404 90025
+ wtd_mean_FusionHeat              1      2865 6294418 90026
+ wtd_std_ElectronAffinity         1      2609 6294674 90026
+ gmean_atomic_mass                1      2546 6294737 90026
+ gmean_FusionHeat                 1      2287 6294995 90027
+ std_FusionHeat                   1      2107 6295176 90027
+ mean_Valence                     1      1712 6295571 90028
+ std_Density                      1      1647 6295636 90028
+ wtd_entropy_FusionHeat           1      1609 6295674 90028
+ mean_ThermalConductivity         1      1325 6295958 90029
+ entropy_FusionHeat               1      1029 6296253 90030
+ entropy_Valence                  1       914 6296368 90030
<none>                                       6297283 90030
+ mean_FusionHeat                 1       829 6296454 90030
+ std_ElectronAffinity            1       733 6296550 90031
+ std_fie                         1       714 6296569 90031
+ gmean_ThermalConductivity       1       621 6296661 90031
+ range_Density                   1       214 6297069 90032
+ mean_atomic_mass                1       178 6297105 90032
+ range_ElectronAffinity          1        55 6297228 90032
+ wtd_range_fie                   1        19 6297264 90032
+ wtd_std_atomic_mass             1        16 6297267 90032

Step:  AIC=89785.72
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density

                                  Df Sum of Sq     RSS   AIC
+ range_atomic_mass                1    151132 6042692 89420
+ wtd_entropy_ThermalConductivity  1    117817 6076006 89502
+ std_atomic_mass                  1    112849 6080975 89514
+ entropy_ThermalConductivity      1     96011 6097813 89555
+ wtd_range_Valence                1     91120 6102703 89567
+ wtd_std_fie                      1     69854 6123970 89619
+ wtd_mean_ThermalConductivity     1     67898 6125926 89624
+ wtd_std_atomic_radius            1     65450 6128373 89630
+ wtd_mean_ElectronAffinity        1     54578 6139246 89656
+ wtd_range_Density                1     51225 6142599 89664
+ wtd_range_atomic_mass            1     50626 6143198 89666
+ range_Valence                    1     45600 6148224 89678
+ wtd_gmean_atomic_radius          1     45283 6148540 89679
+ wtd_entropy_fie                  1     42097 6151726 89686
```

```
+ wtd_mean_atomic_radius           1     37663 6156160 89697
+ wtd_mean_fie                     1     36339 6157484 89700
+ number_of_elements               1     34283 6159541 89705
+ wtd_range_FusionHeat             1     31700 6162124 89711
+ entropy_atomic_mass              1     31284 6162540 89712
+ wtd_gmean_FusionHeat             1     30733 6163090 89714
+ wtd_entropy_FusionHeat           1     30001 6163823 89715
+ wtd_range_ThermalConductivity    1     29062 6164761 89718
+ entropy_fie                      1     27315 6166509 89722
+ std_ThermalConductivity          1     25618 6168206 89726
+ wtd_mean_Valence                 1     25330 6168494 89727
+ std_Valence                      1     24459 6169365 89729
+ wtd_gmean_fie                    1     24119 6169704 89730
+ wtd_gmean_Valence                1     21846 6171977 89735
+ wtd_mean_FusionHeat              1     20373 6173451 89739
+ wtd_mean_atomic_mass             1     19647 6174177 89740
+ entropy_atomic_radius            1     19517 6174307 89741
+ range_ThermalConductivity        1     19343 6174480 89741
+ wtd_range_ElectronAffinity       1     19273 6174551 89741
+ wtd_gmean_atomic_mass            1     18999 6174824 89742
+ wtd_entropy_ElectronAffinity     1     16305 6177518 89748
+ wtd_gmean_Density                1     15805 6178019 89750
+ wtd_entropy_atomic_radius        1     12555 6181269 89758
+ entropy_FusionHeat               1     12176 6181648 89758
+ wtd_mean_Density                 1     11594 6182229 89760
+ wtd_range_atomic_radius          1     11457 6182366 89760
+ wtd_std_atomic_mass              1     10343 6183481 89763
+ wtd_gmean_ThermalConductivity    1      8725 6185099 89767
+ entropy_Valence                  1      7440 6186384 89770
+ wtd_range_fie                    1      7168 6186655 89770
+ mean_ElectronAffinity            1      7116 6186708 89771
+ mean_ThermalConductivity         1      6964 6186860 89771
+ gmean_atomic_radius              1      6782 6187042 89771
+ mean_atomic_radius               1      5924 6187899 89773
+ gmean_fie                        1      5437 6188387 89775
+ wtd_std_Density                  1      4555 6189268 89777
+ mean_FusionHeat                  1      4547 6189277 89777
+ mean_fie                         1      3824 6189999 89779
+ std_fie                          1      3695 6190129 89779
+ wtd_std_FusionHeat               1      3658 6190166 89779
+ std_Density                      1      3522 6190302 89779
+ mean_Density                     1      3395 6190429 89780
+ mean_atomic_mass                 1      2723 6191100 89781
+ gmean_Density                    1      2458 6191365 89782
+ wtd_std_ElectronAffinity         1      2291 6191533 89782
+ gmean_FusionHeat                 1      1893 6191930 89783
+ std_FusionHeat                   1      1651 6192173 89784
+ entropy_Density                  1      1202 6192621 89785
```

```
+ range_Density                    1      1126 6192698 89785
+ gmean_atomic_mass                1      1051 6192772 89785
<none>                                       6193824 89786
+ std_ElectronAffinity             1       744 6193080 89786
+ wtd_entropy_Valence              1       420 6193404 89787
+ gmean_ThermalConductivity        1       349 6193474 89787
+ range_FusionHeat                 1       274 6193550 89787
+ gmean_Valence                    1       261 6193563 89787
+ range_ElectronAffinity           1       251 6193572 89787
+ range_fie                        1       115 6193709 89787
+ mean_Valence                     1        10 6193814 89788

Step:  AIC=89420.04
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass

                                  Df Sum of Sq     RSS   AIC
+ wtd_std_atomic_mass              1    220256 5822436 88869
+ wtd_std_Density                  1    127003 5915689 89106
+ wtd_entropy_ThermalConductivity  1    108512 5934180 89152
+ entropy_ThermalConductivity      1    103337 5939355 89165
+ wtd_std_fie                      1     94534 5948157 89187
+ wtd_range_Valence                1     92159 5950532 89193
+ wtd_std_atomic_radius            1     65525 5977167 89260
+ range_Density                    1     62411 5980281 89268
+ wtd_mean_ThermalConductivity     1     61795 5980897 89269
+ wtd_mean_fie                     1     54798 5987894 89286
+ std_Density                      1     54622 5988069 89287
+ wtd_gmean_atomic_radius          1     51734 5990958 89294
+ mean_Density                     1     43904 5998788 89314
+ wtd_mean_atomic_radius           1     41613 6001079 89319
+ range_Valence                    1     41053 6001639 89321
+ wtd_gmean_fie                    1     39100 6003592 89325
+ std_ThermalConductivity          1     36496 6006196 89332
+ wtd_range_FusionHeat             1     36453 6006239 89332
+ wtd_entropy_fie                  1     35405 6007286 89335
+ range_ThermalConductivity        1     31741 6010951 89344
+ wtd_gmean_FusionHeat             1     30684 6012008 89346
+ wtd_mean_ElectronAffinity        1     30655 6012036 89346
+ std_atomic_mass                  1     27801 6014890 89353
+ wtd_range_ThermalConductivity    1     25555 6017137 89359
+ wtd_mean_FusionHeat              1     22187 6020504 89367
+ std_Valence                      1     21997 6020695 89368
+ wtd_entropy_ElectronAffinity     1     19022 6023670 89375
+ wtd_mean_Valence                 1     18200 6024492 89377
+ wtd_range_Density                1     18126 6024566 89377
```

```
+ number_of_elements               1     17287 6025405 89379
+ entropy_fie                      1     15902 6026790 89383
+ wtd_gmean_Valence                1     15109 6027583 89385
+ mean_atomic_mass                 1     14510 6028182 89386
+ wtd_range_atomic_radius          1     14112 6028580 89387
+ wtd_entropy_FusionHeat           1     13548 6029144 89389
+ wtd_range_ElectronAffinity       1     13138 6029554 89390
+ wtd_range_atomic_mass            1     12779 6029913 89391
+ wtd_gmean_atomic_mass            1     12674 6030018 89391
+ wtd_range_fie                    1     12374 6030318 89392
+ std_fie                          1     12129 6030563 89392
+ entropy_Density                  1     11998 6030694 89392
+ entropy_atomic_radius            1     10706 6031986 89396
+ wtd_gmean_Density                1     10200 6032492 89397
+ gmean_atomic_mass                1      9656 6033036 89398
+ entropy_FusionHeat               1      9287 6033405 89399
+ gmean_Density                    1      8406 6034286 89401
+ mean_atomic_radius               1      8135 6034557 89402
+ gmean_atomic_radius              1      7792 6034899 89403
+ wtd_entropy_Valence              1      7783 6034909 89403
+ wtd_std_ElectronAffinity         1      6819 6035873 89405
+ mean_ThermalConductivity         1      5945 6036747 89407
+ wtd_gmean_ThermalConductivity    1      5430 6037262 89409
+ mean_FusionHeat                  1      5165 6037527 89409
+ gmean_Valence                    1      3588 6039104 89413
+ std_FusionHeat                   1      3551 6039140 89413
+ entropy_Valence                  1      2313 6040379 89416
+ mean_ElectronAffinity            1      2090 6040602 89417
+ wtd_std_FusionHeat               1      1981 6040711 89417
+ gmean_fie                        1      1933 6040758 89417
+ range_ElectronAffinity           1      1919 6040772 89417
+ wtd_mean_atomic_mass             1      1784 6040908 89418
+ mean_Valence                     1      1745 6040947 89418
+ range_fie                        1      1409 6041283 89419
+ range_FusionHeat                 1      1383 6041309 89419
+ gmean_FusionHeat                 1      1257 6041435 89419
<none>                                       6042692 89420
+ mean_fie                        1       806 6041886 89420
+ gmean_ThermalConductivity       1       589 6042102 89421
+ wtd_mean_Density                1       357 6042335 89421
+ wtd_entropy_atomic_radius       1       160 6042532 89422
+ entropy_atomic_mass             1        85 6042607 89422
+ std_ElectronAffinity            1        21 6042671 89422

Step:  AIC=88869.38
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
```

```
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass

                                  Df Sum of Sq     RSS   AIC
+ wtd_entropy_ThermalConductivity  1    102179 5720257 88608
+ wtd_entropy_atomic_radius        1     63312 5759124 88709
+ wtd_entropy_fie                  1     55769 5766667 88728
+ wtd_entropy_FusionHeat           1     55424 5767012 88729
+ entropy_ThermalConductivity      1     46209 5776228 88753
+ range_Density                    1     41330 5781106 88765
+ range_ThermalConductivity        1     35430 5787006 88781
+ std_ThermalConductivity          1     30767 5791669 88793
+ std_Density                      1     30017 5792419 88794
+ mean_Density                     1     29276 5793160 88796
+ wtd_std_Density                  1     27723 5794713 88800
+ wtd_gmean_atomic_radius          1     25835 5796602 88805
+ wtd_mean_atomic_radius           1     25789 5796647 88805
+ wtd_std_fie                      1     25753 5796683 88805
+ wtd_range_fie                    1     23672 5798764 88811
+ wtd_mean_ElectronAffinity        1     23365 5799071 88812
+ wtd_mean_fie                     1     21827 5800609 88815
+ wtd_range_Valence                1     20863 5801574 88818
+ wtd_gmean_fie                    1     17128 5805308 88828
+ wtd_mean_ThermalConductivity     1     16088 5806349 88830
+ entropy_FusionHeat               1     10989 5811447 88843
+ wtd_range_atomic_mass            1     10447 5811989 88845
+ wtd_mean_Valence                 1      9883 5812553 88846
+ wtd_gmean_atomic_mass            1      9699 5812737 88847
+ gmean_Density                    1      9267 5813169 88848
+ gmean_atomic_radius              1      8981 5813455 88848
+ wtd_mean_atomic_mass             1      8924 5813512 88849
+ wtd_range_Density                1      8407 5814029 88850
+ mean_atomic_radius               1      7964 5814472 88851
+ wtd_gmean_Valence                1      7852 5814584 88851
+ wtd_gmean_FusionHeat             1      7735 5814701 88852
+ wtd_std_FusionHeat               1      6751 5815685 88854
+ wtd_std_atomic_radius            1      6150 5816286 88856
+ wtd_entropy_Valence              1      6057 5816379 88856
+ mean_atomic_mass                 1      5935 5816501 88856
+ gmean_atomic_mass                1      4687 5817749 88859
+ wtd_gmean_Density                1      3900 5818536 88861
+ gmean_fie                        1      3874 5818563 88861
+ entropy_fie                      1      3727 5818709 88862
+ wtd_mean_FusionHeat              1      3528 5818908 88862
+ wtd_range_FusionHeat             1      3431 5819005 88863
+ range_Valence                    1      3065 5819372 88864
+ entropy_atomic_mass              1      3016 5819420 88864
+ mean_fie                         1      2906 5819530 88864
+ wtd_std_ElectronAffinity         1      2560 5819876 88865
```

```
+ std_fie                          1      2470 5819966 88865
+ range_ElectronAffinity           1      2425 5820011 88865
+ range_FusionHeat                 1      2247 5820190 88866
+ gmean_Valence                    1      2030 5820406 88866
+ wtd_range_atomic_radius          1      2007 5820430 88866
+ number_of_elements               1      1934 5820502 88866
+ mean_Valence                     1      1911 5820526 88866
+ wtd_mean_Density                 1      1727 5820709 88867
+ gmean_ThermalConductivity        1      1380 5821056 88868
+ mean_ElectronAffinity            1      1316 5821120 88868
+ wtd_entropy_ElectronAffinity     1      1301 5821135 88868
+ entropy_atomic_radius            1      1286 5821150 88868
+ entropy_Valence                  1       988 5821448 88869
+ wtd_range_ElectronAffinity       1       987 5821449 88869
+ mean_FusionHeat                  1       835 5821601 88869
<none>                                       5822436 88869
+ std_FusionHeat                   1       751 5821686 88869
+ std_atomic_mass                  1       727 5821709 88870
+ gmean_FusionHeat                 1       680 5821756 88870
+ wtd_gmean_ThermalConductivity    1       586 5821850 88870
+ wtd_range_ThermalConductivity    1       338 5822098 88871
+ mean_ThermalConductivity         1       205 5822231 88871
+ range_fie                        1       204 5822232 88871
+ std_ElectronAffinity             1       114 5822322 88871
+ entropy_Density                  1        22 5822415 88871
+ std_Valence                      1         0 5822436 88871

Step:  AIC=88607.86
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity

                              Df Sum of Sq     RSS   AIC
+ range_Density                1     68850 5651407 88430
+ range_ThermalConductivity    1     59987 5660270 88453
+ std_Density                  1     57909 5662348 88458
+ wtd_std_Density              1     56659 5663597 88462
+ std_ThermalConductivity      1     52968 5667289 88471
+ mean_ThermalConductivity     1     46096 5674161 88489
+ gmean_ThermalConductivity    1     43247 5677010 88497
+ wtd_std_FusionHeat           1     29381 5690876 88533
+ wtd_entropy_FusionHeat       1     26036 5694221 88542
+ wtd_entropy_fie              1     25191 5695066 88544
+ mean_Density                 1     24196 5696061 88547
+ wtd_mean_atomic_radius       1     22762 5697495 88551
+ wtd_gmean_atomic_radius      1     20643 5699614 88556
```

```
+ wtd_range_Valence               1     19517 5700740 88559
+ range_FusionHeat                1     19483 5700774 88559
+ wtd_gmean_atomic_mass           1     17437 5702820 88564
+ wtd_std_fie                     1     17031 5703226 88565
+ wtd_mean_fie                    1     16882 5703374 88566
+ wtd_mean_atomic_mass            1     16728 5703529 88566
+ wtd_entropy_atomic_radius       1     16670 5703587 88566
+ wtd_range_fie                   1     15692 5704565 88569
+ wtd_gmean_fie                   1     13827 5706430 88574
+ std_FusionHeat                  1     13403 5706854 88575
+ wtd_mean_ElectronAffinity       1     13275 5706982 88575
+ wtd_gmean_ThermalConductivity   1     11456 5708800 88580
+ wtd_mean_Valence                1     10757 5709500 88582
+ wtd_range_atomic_mass           1      9413 5710844 88585
+ gmean_Density                   1      9326 5710931 88586
+ wtd_gmean_Valence               1      8875 5711382 88587
+ wtd_entropy_ElectronAffinity    1      7099 5713158 88591
+ wtd_range_Density               1      5583 5714673 88595
+ mean_FusionHeat                 1      5381 5714876 88596
+ entropy_atomic_mass             1      5297 5714959 88596
+ wtd_range_ThermalConductivity   1      5079 5715178 88597
+ gmean_FusionHeat                1      4862 5715395 88597
+ range_ElectronAffinity          1      4705 5715552 88598
+ wtd_mean_ThermalConductivity    1      4041 5716216 88599
+ gmean_atomic_radius             1      4036 5716221 88599
+ range_Valence                   1      4005 5716252 88599
+ gmean_fie                       1      3699 5716558 88600
+ wtd_std_ElectronAffinity        1      3489 5716768 88601
+ wtd_std_atomic_radius           1      3326 5716931 88601
+ entropy_FusionHeat              1      3063 5717193 88602
+ mean_fie                        1      2930 5717327 88602
+ mean_atomic_radius              1      2706 5717551 88603
+ wtd_range_ElectronAffinity      1      2128 5718129 88604
+ wtd_gmean_Density               1      1831 5718426 88605
+ entropy_atomic_radius           1      1830 5718427 88605
+ wtd_range_atomic_radius         1      1590 5718667 88606
+ std_fie                         1      1409 5718848 88606
+ std_Valence                     1      1293 5718964 88606
+ entropy_Valence                 1      1081 5719175 88607
+ std_ElectronAffinity            1       903 5719353 88608
+ std_atomic_mass                 1       769 5719487 88608
<none>                                       5720257 88608
+ wtd_mean_Density                1       756 5719501 88608
+ range_fie                       1       579 5719678 88608
+ wtd_range_FusionHeat            1       475 5719782 88609
+ wtd_mean_FusionHeat             1       339 5719918 88609
+ entropy_Density                 1       309 5719948 88609
+ entropy_fie                     1       290 5719967 88609
```

```
+ gmean_atomic_mass              1       260 5719996 88609
+ wtd_entropy_Valence            1       177 5720080 88609
+ mean_atomic_mass               1       135 5720122 88610
+ wtd_gmean_FusionHeat           1       124 5720133 88610
+ entropy_ThermalConductivity    1        73 5720184 88610
+ number_of_elements             1        54 5720203 88610
+ gmean_Valence                  1         4 5720252 88610
+ mean_Valence                   1         1 5720256 88610
+ mean_ElectronAffinity          1         0 5720257 88610

Step:  AIC=88429.63
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density

                              Df Sum of Sq     RSS   AIC
+ range_ThermalConductivity    1     62220 5589186 88267
+ std_ThermalConductivity      1     54641 5596766 88287
+ wtd_mean_atomic_radius       1     41485 5609922 88322
+ mean_ThermalConductivity     1     37497 5613910 88333
+ wtd_gmean_atomic_radius      1     36514 5614893 88335
+ gmean_ThermalConductivity    1     34369 5617038 88341
+ wtd_range_Valence            1     33893 5617514 88342
+ wtd_range_Density            1     29606 5621801 88353
+ wtd_std_FusionHeat           1     26910 5624496 88361
+ wtd_mean_Valence             1     26349 5625058 88362
+ wtd_mean_atomic_mass         1     24958 5626448 88366
+ wtd_gmean_atomic_mass        1     24788 5626619 88366
+ wtd_entropy_fie              1     24472 5626935 88367
+ wtd_gmean_Valence            1     23446 5627960 88370
+ wtd_entropy_FusionHeat       1     22599 5628807 88372
+ wtd_std_fie                  1     20353 5631054 88378
+ wtd_range_atomic_mass        1     18748 5632659 88382
+ range_FusionHeat             1     16934 5634473 88387
+ range_Valence                1     16539 5634867 88388
+ wtd_mean_fie                 1     14324 5637083 88394
+ wtd_mean_Density             1     14314 5637093 88394
+ std_Valence                  1     13467 5637940 88396
+ wtd_mean_ElectronAffinity    1     13372 5638034 88396
+ std_FusionHeat               1     11927 5639480 88400
+ wtd_gmean_fie                1     10625 5640782 88404
+ wtd_range_fie                1      9955 5641452 88405
+ wtd_gmean_Density            1      9282 5642125 88407
+ mean_Valence                 1      9235 5642172 88407
+ gmean_fie                    1      8913 5642494 88408
+ wtd_range_ThermalConductivity 1     8904 5642503 88408
```

```
+ wtd_entropy_atomic_radius      1      8728 5642678 88409
+ wtd_entropy_ElectronAffinity   1      8283 5643124 88410
+ wtd_gmean_ThermalConductivity  1      7151 5644256 88413
+ wtd_mean_ThermalConductivity   1      7114 5644293 88413
+ gmean_Valence                  1      6972 5644435 88413
+ mean_fie                       1      6642 5644765 88414
+ wtd_range_ElectronAffinity     1      6115 5645292 88416
+ entropy_FusionHeat             1      4133 5647274 88421
+ std_Density                    1      3683 5647724 88422
+ range_ElectronAffinity         1      3309 5648098 88423
+ mean_atomic_mass               1      3268 5648139 88423
+ gmean_atomic_mass              1      3139 5648268 88423
+ entropy_ThermalConductivity    1      2920 5648487 88424
+ std_fie                        1      2682 5648725 88425
+ mean_FusionHeat                1      2426 5648981 88425
+ wtd_std_ElectronAffinity       1      2116 5649290 88426
+ gmean_FusionHeat               1      1618 5649789 88427
+ entropy_atomic_mass            1      1324 5650083 88428
+ entropy_Density                1      1007 5650400 88429
+ wtd_std_atomic_radius          1       837 5650570 88429
<none>                                      5651407 88430
+ wtd_range_FusionHeat           1       547 5650860 88430
+ wtd_entropy_Valence            1       541 5650865 88430
+ gmean_Density                  1       464 5650943 88430
+ mean_Density                   1       412 5650995 88431
+ wtd_gmean_FusionHeat           1       290 5651117 88431
+ wtd_range_atomic_radius        1       240 5651167 88431
+ wtd_mean_FusionHeat            1       215 5651192 88431
+ entropy_Valence                1       180 5651227 88431
+ std_ElectronAffinity           1       146 5651261 88431
+ entropy_fie                    1       140 5651267 88431
+ entropy_atomic_radius          1       138 5651269 88431
+ wtd_std_Density                1       134 5651273 88431
+ mean_ElectronAffinity          1        80 5651327 88431
+ std_atomic_mass                1        75 5651332 88431
+ gmean_atomic_radius            1        40 5651366 88432
+ number_of_elements             1        30 5651377 88432
+ mean_atomic_radius             1         6 5651400 88432
+ range_fie                      1         1 5651406 88432

Step:  AIC=88266.85
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity

                                Df Sum of Sq     RSS   AIC
```

```
+ gmean_ThermalConductivity      1     40765 5548421 88160
+ wtd_range_Valence              1     39119 5550067 88164
+ wtd_std_FusionHeat             1     38890 5550296 88165
+ wtd_entropy_ElectronAffinity   1     32665 5556522 88182
+ range_Valence                  1     27346 5561840 88196
+ wtd_entropy_FusionHeat         1     27264 5561923 88196
+ wtd_mean_ElectronAffinity      1     25725 5563461 88200
+ std_Valence                    1     25165 5564021 88202
+ wtd_range_ElectronAffinity     1     24890 5564297 88202
+ range_FusionHeat               1     22322 5566865 88209
+ std_FusionHeat                 1     16981 5572206 88224
+ wtd_range_Density              1     16007 5573179 88226
+ wtd_gmean_ThermalConductivity  1     14825 5574361 88229
+ gmean_fie                      1     13148 5576038 88234
+ wtd_range_atomic_mass          1     13135 5576052 88234
+ wtd_mean_Valence               1     12496 5576690 88236
+ wtd_mean_atomic_radius         1     12085 5577102 88237
+ mean_fie                       1     11658 5577529 88238
+ mean_ThermalConductivity       1     11571 5577616 88238
+ wtd_gmean_Valence              1     10888 5578299 88240
+ wtd_mean_atomic_mass           1     10497 5578690 88241
+ wtd_gmean_atomic_mass          1     10306 5578881 88241
+ mean_FusionHeat                1      8921 5580265 88245
+ gmean_FusionHeat               1      8423 5580763 88246
+ wtd_gmean_atomic_radius        1      8321 5580865 88247
+ wtd_entropy_atomic_radius      1      5619 5583568 88254
+ gmean_Density                  1      5149 5584038 88255
+ wtd_std_Density                1      5139 5584048 88255
+ entropy_Density                1      4121 5585066 88258
+ wtd_mean_FusionHeat            1      4089 5585098 88258
+ entropy_ThermalConductivity    1      3680 5585507 88259
+ wtd_std_fie                    1      2633 5586553 88262
+ gmean_atomic_radius            1      2631 5586555 88262
+ mean_Valence                   1      2272 5586915 88263
+ wtd_entropy_fie                1      2161 5587025 88263
+ mean_ElectronAffinity          1      2145 5587042 88263
+ mean_Density                   1      2120 5587066 88263
+ std_Density                    1      2025 5587162 88263
+ range_ElectronAffinity         1      1886 5587300 88264
+ wtd_range_fie                  1      1784 5587402 88264
+ wtd_mean_Density               1      1771 5587416 88264
+ wtd_entropy_Valence            1      1666 5587521 88264
+ mean_atomic_radius             1      1597 5587589 88265
+ range_fie                      1      1587 5587599 88265
+ entropy_FusionHeat             1      1564 5587622 88265
+ gmean_atomic_mass              1      1208 5587978 88266
+ mean_atomic_mass               1      1109 5588077 88266
+ wtd_std_atomic_radius          1      1065 5588121 88266
```

```
+ wtd_gmean_FusionHeat           1      1038 5588148 88266
+ gmean_Valence                  1      1031 5588156 88266
+ wtd_std_ElectronAffinity       1       917 5588269 88266
+ wtd_gmean_Density              1       772 5588415 88267
+ std_atomic_mass                1       768 5588418 88267
<none>                                      5589186 88267
+ entropy_atomic_mass            1       460 5588727 88268
+ wtd_range_atomic_radius        1       382 5588805 88268
+ entropy_fie                    1       280 5588906 88268
+ wtd_range_ThermalConductivity  1       229 5588957 88268
+ entropy_Valence                1       223 5588964 88268
+ wtd_gmean_fie                  1       121 5589065 88269
+ entropy_atomic_radius          1        43 5589144 88269
+ std_ThermalConductivity        1        25 5589162 88269
+ number_of_elements             1        11 5589176 88269
+ std_ElectronAffinity           1         8 5589179 88269
+ std_fie                        1         4 5589182 88269
+ wtd_mean_ThermalConductivity   1         3 5589184 88269
+ wtd_range_FusionHeat           1         1 5589185 88269
+ wtd_mean_fie                   1         1 5589186 88269

Step:  AIC=88159.89
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity

                                Df Sum of Sq     RSS   AIC
+ wtd_entropy_ElectronAffinity   1     45044 5503377 88041
+ wtd_range_Valence              1     39284 5509137 88056
+ wtd_mean_ThermalConductivity   1     36264 5512157 88064
+ std_Valence                    1     29554 5518867 88082
+ range_Valence                  1     29418 5519003 88083
+ wtd_range_ElectronAffinity     1     24490 5523932 88096
+ wtd_std_FusionHeat             1     23818 5524604 88098
+ wtd_range_Density              1     23238 5525183 88099
+ wtd_entropy_FusionHeat         1     20809 5527612 88106
+ wtd_mean_ElectronAffinity      1     18773 5529648 88111
+ mean_ThermalConductivity       1     17745 5530677 88114
+ wtd_range_ThermalConductivity  1     12862 5535559 88127
+ range_FusionHeat               1     11619 5536802 88131
+ wtd_mean_atomic_radius         1      9555 5538866 88136
+ wtd_std_fie                    1      9030 5539391 88138
+ wtd_range_atomic_mass          1      8789 5539632 88138
+ wtd_mean_Valence               1      8710 5539711 88139
```

```
+ wtd_gmean_Valence              1      7449 5540972 88142
+ gmean_fie                      1      7331 5541090 88142
+ wtd_gmean_atomic_radius        1      6937 5541484 88143
+ std_FusionHeat                 1      6807 5541614 88144
+ wtd_entropy_Valence            1      6339 5542082 88145
+ wtd_gmean_ThermalConductivity  1      6182 5542239 88145
+ mean_fie                       1      5556 5542865 88147
+ wtd_range_FusionHeat           1      5454 5542967 88147
+ wtd_std_Density                1      5174 5543247 88148
+ range_ElectronAffinity         1      4892 5543529 88149
+ wtd_mean_atomic_mass           1      4256 5544165 88150
+ wtd_gmean_atomic_mass          1      4193 5544228 88151
+ wtd_std_ElectronAffinity       1      3816 5544605 88152
+ wtd_mean_Density               1      3607 5544815 88152
+ wtd_gmean_FusionHeat           1      3489 5544933 88153
+ wtd_range_fie                  1      3427 5544994 88153
+ wtd_gmean_Density              1      3396 5545026 88153
+ entropy_FusionHeat             1      3075 5545346 88154
+ std_Density                    1      2804 5545617 88154
+ std_fie                        1      2034 5546387 88156
+ gmean_Density                  1      1664 5546757 88157
+ wtd_entropy_atomic_radius      1      1652 5546769 88157
+ entropy_atomic_mass            1      1600 5546821 88158
+ mean_Valence                   1      1433 5546988 88158
+ entropy_Valence                1      1348 5547074 88158
+ gmean_atomic_radius            1      1190 5547232 88159
<none>                                     5548421 88160
+ mean_Density                   1       717 5547705 88160
+ mean_atomic_radius             1       659 5547762 88160
+ mean_ElectronAffinity          1       557 5547864 88160
+ std_ElectronAffinity           1       475 5547946 88161
+ gmean_Valence                  1       461 5547961 88161
+ wtd_mean_FusionHeat            1       404 5548017 88161
+ entropy_Density                1       392 5548029 88161
+ wtd_range_atomic_radius        1       363 5548058 88161
+ wtd_std_atomic_radius          1       361 5548060 88161
+ mean_FusionHeat                1       361 5548060 88161
+ entropy_atomic_radius          1       266 5548155 88161
+ gmean_FusionHeat               1       264 5548157 88161
+ entropy_ThermalConductivity    1       122 5548299 88162
+ wtd_mean_fie                   1        87 5548334 88162
+ mean_atomic_mass               1        77 5548345 88162
+ wtd_entropy_fie                1        64 5548357 88162
+ number_of_elements             1        48 5548373 88162
+ wtd_gmean_fie                  1        47 5548375 88162
+ gmean_atomic_mass              1        34 5548387 88162
+ std_ThermalConductivity        1        21 5548400 88162
+ entropy_fie                    1        11 5548411 88162
```

```
+ std_atomic_mass                1         7 5548414 88162
+ range_fie                      1         2 5548419 88162

Step:  AIC=88040.57
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity

                               Df Sum of Sq     RSS   AIC
+ wtd_mean_ThermalConductivity   1     48215 5455162 87912
+ wtd_entropy_FusionHeat         1     29877 5473501 87962
+ gmean_fie                      1     25630 5477748 87973
+ wtd_std_FusionHeat             1     24944 5478433 87975
+ wtd_range_Density              1     24549 5478828 87976
+ mean_fie                       1     24392 5478985 87976
+ range_Valence                  1     23257 5480120 87980
+ wtd_range_Valence              1     23144 5480234 87980
+ mean_ThermalConductivity       1     23028 5480349 87980
+ wtd_entropy_fie                1     22701 5480676 87981
+ std_Valence                    1     19000 5484377 87991
+ wtd_range_ThermalConductivity  1     17043 5486334 87996
+ range_FusionHeat               1     12066 5491311 88010
+ wtd_mean_atomic_radius         1     11543 5491835 88011
+ wtd_gmean_ThermalConductivity  1     11009 5492369 88013
+ wtd_mean_ElectronAffinity      1     10276 5493101 88015
+ wtd_range_atomic_mass          1      9355 5494022 88017
+ wtd_gmean_atomic_radius        1      8966 5494412 88018
+ gmean_atomic_radius            1      7960 5495417 88021
+ std_FusionHeat                 1      7674 5495703 88022
+ mean_ElectronAffinity          1      7578 5495799 88022
+ wtd_mean_Valence               1      6931 5496446 88024
+ wtd_mean_Density               1      6472 5496905 88025
+ wtd_entropy_atomic_radius      1      6055 5497323 88026
+ range_fie                      1      5987 5497390 88026
+ wtd_mean_atomic_mass           1      5943 5497434 88026
+ mean_atomic_radius             1      5777 5497600 88027
+ wtd_gmean_Valence              1      5746 5497631 88027
+ wtd_gmean_atomic_mass          1      5738 5497640 88027
+ wtd_std_Density                1      4839 5498538 88029
+ wtd_std_fie                    1      4154 5499223 88031
+ std_Density                    1      3952 5499425 88032
+ gmean_Density                  1      3659 5499718 88033
+ wtd_std_ElectronAffinity       1      3391 5499987 88033
+ wtd_gmean_Density              1      3358 5500020 88033
```

```
+ wtd_range_ElectronAffinity     1      3011 5500366 88034
+ entropy_FusionHeat             1      2544 5500834 88036
+ wtd_range_FusionHeat           1      1925 5501453 88037
+ wtd_gmean_FusionHeat           1      1726 5501652 88038
+ entropy_Density                1      1709 5501668 88038
+ std_ElectronAffinity           1      1439 5501938 88039
+ mean_Density                   1      1408 5501969 88039
+ std_atomic_mass                1      1144 5502233 88039
+ entropy_fie                    1      1118 5502259 88040
+ gmean_FusionHeat               1       922 5502455 88040
+ entropy_atomic_mass            1       857 5502521 88040
+ mean_FusionHeat                1       820 5502558 88040
<none>                                     5503377 88041
+ std_fie                        1       738 5502639 88041
+ wtd_range_fie                  1       723 5502654 88041
+ gmean_atomic_mass              1       351 5503026 88042
+ mean_atomic_mass               1       347 5503030 88042
+ mean_Valence                   1       327 5503051 88042
+ wtd_std_atomic_radius          1       282 5503095 88042
+ wtd_entropy_Valence            1       273 5503105 88042
+ wtd_mean_fie                   1       217 5503160 88042
+ std_ThermalConductivity        1       196 5503181 88042
+ wtd_range_atomic_radius        1       176 5503201 88042
+ number_of_elements             1       171 5503206 88042
+ entropy_atomic_radius          1        33 5503344 88042
+ wtd_mean_FusionHeat            1        32 5503345 88042
+ range_ElectronAffinity         1        27 5503350 88042
+ gmean_Valence                  1        20 5503357 88043
+ entropy_ThermalConductivity    1         8 5503369 88043
+ entropy_Valence                1         5 5503372 88043
+ wtd_gmean_fie                  1         1 5503377 88043

Step:  AIC=87911.6
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity

                                Df Sum of Sq     RSS   AIC
+ wtd_gmean_ThermalConductivity  1     52945 5402217 87768
+ wtd_entropy_FusionHeat         1     36367 5418796 87814
+ wtd_std_FusionHeat             1     29555 5425608 87833
+ gmean_fie                      1     26814 5428348 87840
+ wtd_range_Valence              1     25886 5429276 87843
```

```
+ range_Valence                  1     25222 5429941 87845
+ mean_fie                       1     25081 5430081 87845
+ std_Valence                    1     20908 5434254 87856
+ range_FusionHeat               1     17234 5437929 87867
+ wtd_range_ThermalConductivity  1     16079 5439083 87870
+ std_FusionHeat                 1     12202 5442960 87880
+ wtd_range_Density              1     11415 5443748 87882
+ mean_ThermalConductivity       1     10930 5444233 87884
+ wtd_entropy_atomic_radius      1      8846 5446317 87889
+ gmean_atomic_radius            1      8482 5446680 87890
+ wtd_std_atomic_radius          1      6860 5448302 87895
+ wtd_gmean_fie                  1      6615 5448548 87896
+ mean_atomic_radius             1      6046 5449116 87897
+ mean_ElectronAffinity          1      5832 5449331 87898
+ wtd_mean_fie                   1      5751 5449411 87898
+ wtd_range_atomic_mass          1      5731 5449432 87898
+ wtd_std_ElectronAffinity       1      5713 5449450 87898
+ wtd_mean_Valence               1      5400 5449762 87899
+ range_fie                      1      5340 5449822 87899
+ gmean_Density                  1      5239 5449923 87899
+ wtd_std_Density                1      5016 5450146 87900
+ wtd_mean_ElectronAffinity      1      4854 5450308 87900
+ wtd_gmean_Valence              1      4330 5450833 87902
+ wtd_range_fie                  1      4301 5450861 87902
+ std_atomic_mass                1      3701 5451461 87903
+ entropy_FusionHeat             1      3338 5451825 87904
+ std_Density                    1      3298 5451865 87905
+ wtd_entropy_fie                1      2756 5452407 87906
+ entropy_ThermalConductivity    1      2628 5452534 87906
+ entropy_Density                1      2155 5453008 87908
+ wtd_mean_atomic_radius         1      2070 5453093 87908
+ mean_Density                   1      1616 5453546 87909
+ wtd_mean_atomic_mass           1      1599 5453563 87909
+ entropy_atomic_mass            1      1571 5453591 87909
+ wtd_entropy_Valence            1      1437 5453725 87910
+ wtd_gmean_atomic_mass          1      1291 5453871 87910
+ wtd_mean_FusionHeat            1      1282 5453881 87910
+ mean_FusionHeat                1      1111 5454052 87911
+ mean_atomic_mass               1       934 5454229 87911
+ std_ElectronAffinity           1       913 5454249 87911
+ gmean_atomic_mass              1       873 5454289 87911
<none>                                     5455162 87912
+ wtd_mean_Density              1       729 5454434 87912
+ mean_Valence                  1       586 5454576 87912
+ gmean_FusionHeat              1       485 5454678 87912
+ wtd_gmean_atomic_radius       1       433 5454730 87912
+ std_fie                       1       375 5454788 87913
+ entropy_fie                   1       319 5454843 87913
```

```
+ std_ThermalConductivity        1       275 5454887 87913
+ wtd_range_ElectronAffinity     1       178 5454985 87913
+ range_ElectronAffinity         1       163 5454999 87913
+ entropy_atomic_radius          1       124 5455038 87913
+ entropy_Valence                1       124 5455039 87913
+ gmean_Valence                  1       114 5455048 87913
+ wtd_gmean_Density              1        94 5455069 87913
+ number_of_elements             1        60 5455102 87913
+ wtd_std_fie                    1        10 5455152 87914
+ wtd_range_FusionHeat           1         6 5455157 87914
+ wtd_gmean_FusionHeat           1         2 5455160 87914
+ wtd_range_atomic_radius        1         2 5455160 87914

Step:  AIC=87768.43
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity

                               Df Sum of Sq     RSS   AIC
+ wtd_entropy_FusionHeat         1     50162 5352055 87632
+ wtd_std_FusionHeat             1     34921 5367296 87674
+ range_FusionHeat               1     20214 5382003 87715
+ wtd_range_Valence              1     18764 5383453 87719
+ range_Valence                  1     17499 5384718 87722
+ gmean_fie                      1     16595 5385622 87725
+ mean_fie                       1     15866 5386351 87727
+ std_FusionHeat                 1     15045 5387172 87729
+ std_Valence                    1     13672 5388545 87733
+ wtd_std_ElectronAffinity       1     11585 5390632 87738
+ wtd_range_Density              1     11322 5390895 87739
+ wtd_entropy_atomic_radius      1     11056 5391161 87740
+ wtd_range_fie                  1     10077 5392140 87743
+ wtd_range_ThermalConductivity  1      8765 5393452 87746
+ entropy_ThermalConductivity    1      8432 5393785 87747
+ std_ThermalConductivity        1      7533 5394684 87750
+ wtd_gmean_fie                  1      6925 5395292 87751
+ wtd_mean_fie                   1      6615 5395602 87752
+ wtd_std_Density                1      6015 5396202 87754
+ wtd_range_atomic_mass          1      5602 5396615 87755
+ wtd_std_atomic_radius          1      5204 5397013 87756
+ std_atomic_mass                1      4613 5397604 87758
+ entropy_FusionHeat             1      4530 5397687 87758
+ gmean_atomic_radius            1      4023 5398194 87759
```

```
+ gmean_Density                 1      3346 5398871 87761
+ range_fie                     1      3345 5398872 87761
+ entropy_atomic_mass           1      3072 5399145 87762
+ entropy_Density               1      2889 5399328 87762
+ wtd_entropy_Valence           1      2576 5399641 87763
+ std_Density                   1      2468 5399749 87764
+ mean_atomic_radius            1      2410 5399807 87764
+ number_of_elements            1      2341 5399876 87764
+ wtd_mean_atomic_mass          1      2102 5400115 87765
+ mean_ElectronAffinity         1      1978 5400239 87765
+ wtd_mean_atomic_radius        1      1765 5400452 87766
+ wtd_gmean_atomic_mass         1      1672 5400545 87766
+ wtd_mean_FusionHeat           1      1408 5400809 87767
+ range_ElectronAffinity        1      1324 5400893 87767
+ wtd_mean_Density              1      1298 5400919 87767
+ entropy_atomic_radius         1      1248 5400969 87767
+ mean_FusionHeat               1      1219 5400998 87767
+ wtd_gmean_Density             1      1177 5401040 87767
+ entropy_Valence               1       955 5401262 87768
+ wtd_mean_Valence              1       914 5401303 87768
+ wtd_mean_ElectronAffinity     1       837 5401380 87768
+ mean_Density                  1       820 5401397 87768
+ mean_ThermalConductivity      1       800 5401417 87768
<none>                                     5402217 87768
+ wtd_gmean_Valence             1       594 5401623 87769
+ wtd_gmean_atomic_radius       1       298 5401919 87770
+ gmean_Valence                 1       195 5402022 87770
+ wtd_gmean_FusionHeat          1       178 5402039 87770
+ wtd_range_FusionHeat          1       120 5402097 87770
+ std_fie                       1       108 5402109 87770
+ gmean_FusionHeat              1       107 5402110 87770
+ gmean_atomic_mass             1        71 5402146 87770
+ mean_atomic_mass              1        71 5402146 87770
+ entropy_fie                   1        70 5402147 87770
+ std_ElectronAffinity          1        69 5402148 87770
+ wtd_std_fie                   1        47 5402169 87770
+ wtd_entropy_fie               1        37 5402180 87770
+ mean_Valence                  1        33 5402184 87770
+ wtd_range_atomic_radius       1        15 5402202 87770
+ wtd_range_ElectronAffinity    1         4 5402213 87770

Step:  AIC=87631.58
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
```

```
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat

                                Df Sum of Sq     RSS   AIC
+ wtd_range_Valence              1     33730 5318325 87539
+ wtd_entropy_Valence            1     21457 5330598 87574
+ range_Valence                  1     18648 5333407 87582
+ wtd_std_ElectronAffinity       1     18346 5333709 87582
+ std_ThermalConductivity        1     17520 5334535 87585
+ gmean_fie                      1     16913 5335142 87586
+ mean_fie                       1     16575 5335480 87587
+ wtd_std_FusionHeat             1     16280 5335775 87588
+ std_Valence                    1     15342 5336713 87591
+ wtd_range_fie                  1     13867 5338188 87595
+ range_FusionHeat               1     11253 5340802 87602
+ wtd_range_FusionHeat           1     11019 5341036 87603
+ wtd_std_Density                1     10104 5341951 87605
+ entropy_ThermalConductivity    1      9554 5342501 87607
+ wtd_range_Density              1      6940 5345115 87614
+ std_FusionHeat                 1      6468 5345587 87616
+ gmean_atomic_radius            1      6066 5345989 87617
+ number_of_elements             1      5993 5346062 87617
+ wtd_range_ThermalConductivity  1      5155 5346900 87619
+ gmean_Density                  1      4871 5347184 87620
+ wtd_gmean_fie                  1      4671 5347384 87621
+ mean_atomic_radius             1      4415 5347640 87621
+ entropy_atomic_mass            1      4139 5347916 87622
+ wtd_mean_fie                   1      3699 5348356 87623
+ wtd_std_atomic_radius          1      3354 5348701 87624
+ range_fie                      1      2749 5349306 87626
+ entropy_Density                1      2589 5349466 87626
+ std_Density                    1      2426 5349629 87627
+ wtd_mean_Valence               1      2200 5349855 87627
+ mean_Density                   1      2036 5350019 87628
+ wtd_gmean_FusionHeat           1      1971 5350084 87628
+ wtd_std_fie                    1      1870 5350185 87628
+ mean_FusionHeat                1      1813 5350242 87629
+ wtd_range_atomic_mass          1      1740 5350315 87629
+ entropy_atomic_radius          1      1677 5350378 87629
+ gmean_FusionHeat               1      1639 5350416 87629
+ wtd_gmean_Valence              1      1591 5350464 87629
+ entropy_Valence                1      1548 5350507 87629
+ range_ElectronAffinity         1      1539 5350516 87629
+ wtd_mean_atomic_radius         1      1267 5350788 87630
+ gmean_Valence                  1      1169 5350885 87630
+ mean_ThermalConductivity       1       896 5351159 87631
<none>                                      5352055 87632
```

```
+ gmean_atomic_mass              1       683 5351372 87632
+ mean_ElectronAffinity          1       633 5351422 87632
+ std_atomic_mass                1       612 5351443 87632
+ mean_Valence                   1       569 5351486 87632
+ wtd_range_atomic_radius        1       543 5351512 87632
+ mean_atomic_mass               1       515 5351540 87632
+ wtd_mean_ElectronAffinity      1       489 5351566 87632
+ wtd_entropy_atomic_radius      1       335 5351720 87633
+ wtd_gmean_atomic_radius        1       286 5351769 87633
+ entropy_FusionHeat             1       251 5351804 87633
+ wtd_range_ElectronAffinity     1       230 5351825 87633
+ wtd_mean_FusionHeat            1       219 5351836 87633
+ entropy_fie                    1       156 5351899 87633
+ std_fie                        1       143 5351912 87633
+ wtd_gmean_Density              1       105 5351950 87633
+ wtd_mean_atomic_mass           1        99 5351956 87633
+ wtd_gmean_atomic_mass          1        75 5351980 87633
+ wtd_mean_Density               1        61 5351994 87633
+ std_ElectronAffinity           1         5 5352050 87634
+ wtd_entropy_fie                1         2 5352053 87634

Step:  AIC=87539.48
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence

                                Df Sum of Sq     RSS   AIC
+ wtd_std_ElectronAffinity       1   26785.1 5291540 87466
+ entropy_atomic_mass            1   22373.5 5295951 87479
+ mean_fie                       1   21378.8 5296946 87482
+ gmean_fie                      1   21344.7 5296980 87482
+ wtd_range_ThermalConductivity  1   20560.7 5297764 87484
+ entropy_Density                1   18974.4 5299350 87488
+ wtd_range_atomic_radius        1   17959.3 5300365 87491
+ gmean_Density                  1   17567.2 5300758 87492
+ range_Valence                  1   17444.8 5300880 87493
+ entropy_ThermalConductivity    1   15966.6 5302358 87497
+ gmean_atomic_radius            1   14499.5 5303825 87501
+ wtd_gmean_fie                  1   13104.2 5305220 87505
+ wtd_mean_fie                   1   12454.7 5305870 87507
+ std_Valence                    1   11955.3 5306369 87508
+ std_ThermalConductivity        1   11057.2 5307267 87511
```

```
+ mean_atomic_radius             1   11041.1 5307284 87511
+ wtd_std_atomic_radius          1   10630.6 5307694 87512
+ entropy_atomic_radius          1   10589.4 5307735 87512
+ gmean_Valence                  1   10246.5 5308078 87513
+ entropy_Valence                1    9817.3 5308507 87514
+ wtd_std_FusionHeat             1    9493.3 5308831 87515
+ wtd_range_ElectronAffinity     1    9434.8 5308890 87515
+ wtd_std_Density                1    9404.1 5308921 87515
+ mean_Valence                   1    8691.9 5309633 87517
+ entropy_FusionHeat             1    8642.8 5309682 87517
+ mean_Density                   1    8587.4 5309737 87517
+ range_FusionHeat               1    7178.6 5311146 87521
+ range_ElectronAffinity         1    6347.8 5311977 87524
+ wtd_gmean_Valence              1    5983.4 5312341 87525
+ wtd_entropy_Valence            1    5866.9 5312458 87525
+ number_of_elements             1    5633.5 5312691 87526
+ wtd_mean_Valence               1    5215.4 5313109 87527
+ wtd_entropy_atomic_radius      1    4885.1 5313440 87528
+ entropy_fie                    1    4651.7 5313673 87528
+ range_fie                      1    4641.5 5313683 87528
+ wtd_gmean_Density              1    4072.1 5314253 87530
+ std_FusionHeat                 1    3915.8 5314409 87531
+ wtd_mean_Density               1    3785.8 5314539 87531
+ wtd_range_atomic_mass          1    3610.7 5314714 87531
+ wtd_range_FusionHeat           1    3495.0 5314830 87532
+ gmean_atomic_mass              1    3196.7 5315128 87533
+ std_atomic_mass                1    2949.9 5315375 87533
+ wtd_gmean_atomic_radius        1    2846.9 5315478 87534
+ gmean_FusionHeat               1    2575.9 5315749 87534
+ wtd_range_fie                  1    2347.2 5315977 87535
+ mean_atomic_mass               1    2299.4 5316025 87535
+ std_ElectronAffinity           1    2204.7 5316120 87535
+ mean_FusionHeat                1    1893.3 5316431 87536
+ wtd_mean_ElectronAffinity      1    1346.7 5316978 87538
+ mean_ThermalConductivity       1    1257.1 5317068 87538
+ wtd_gmean_atomic_mass          1    1211.9 5317113 87538
+ wtd_range_Density              1    1170.8 5317154 87538
+ wtd_mean_atomic_mass           1     887.0 5317438 87539
+ std_Density                    1     821.4 5317503 87539
+ wtd_mean_atomic_radius         1     804.9 5317520 87539
+ std_fie                        1     714.9 5317610 87539
<none>                                     5318325 87539
+ wtd_gmean_FusionHeat           1     489.5 5317835 87540
+ mean_ElectronAffinity          1      26.5 5318298 87541
+ wtd_mean_FusionHeat            1      14.0 5318311 87541
+ wtd_entropy_fie                1       1.6 5318323 87541
+ wtd_std_fie                    1       0.5 5318324 87541
```

```
Step:  AIC=87466.33
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity

                               Df Sum of Sq     RSS   AIC
+ wtd_mean_ElectronAffinity     1     41431 5250108 87351
+ mean_fie                      1     39994 5251546 87355
+ gmean_fie                     1     38367 5253173 87360
+ std_ElectronAffinity          1     35689 5255851 87368
+ mean_ElectronAffinity         1     32171 5259368 87378
+ gmean_atomic_radius           1     28407 5263132 87388
+ mean_atomic_radius            1     23747 5267792 87401
+ gmean_Density                 1     20797 5270743 87410
+ wtd_range_ThermalConductivity 1     20744 5270795 87410
+ range_Valence                 1     19393 5272147 87414
+ wtd_mean_fie                  1     17894 5273646 87418
+ wtd_gmean_fie                 1     17660 5273880 87419
+ wtd_std_atomic_radius         1     16550 5274990 87422
+ range_fie                     1     13480 5278059 87430
+ mean_Density                  1     13439 5278101 87430
+ entropy_ThermalConductivity   1     11680 5279859 87435
+ entropy_Density               1     10981 5280559 87437
+ std_Valence                   1     10798 5280741 87438
+ wtd_range_atomic_radius       1     10778 5280762 87438
+ wtd_entropy_atomic_radius     1     10529 5281011 87439
+ gmean_Valence                 1     10459 5281080 87439
+ mean_Valence                  1      9130 5282409 87443
+ std_ThermalConductivity       1      8946 5282594 87443
+ wtd_entropy_fie               1      8935 5282604 87443
+ wtd_std_Density               1      8514 5283026 87444
+ range_ElectronAffinity        1      8060 5283479 87446
+ entropy_atomic_mass           1      7426 5284114 87447
+ gmean_atomic_mass             1      6045 5285494 87451
+ entropy_FusionHeat            1      5239 5286300 87454
+ std_fie                       1      5222 5286317 87454
+ mean_atomic_mass              1      5210 5286329 87454
+ wtd_gmean_Valence             1      4927 5286612 87454
+ wtd_mean_Density              1      4713 5286827 87455
+ wtd_gmean_atomic_radius       1      4666 5286874 87455
+ wtd_gmean_Density             1      4628 5286911 87455
+ std_atomic_mass               1      4507 5287033 87456
```

```
+ wtd_mean_Valence               1      4238 5287301 87456
+ wtd_range_FusionHeat           1      4189 5287351 87457
+ gmean_FusionHeat               1      3951 5287589 87457
+ wtd_std_FusionHeat             1      3208 5288332 87459
+ range_FusionHeat               1      2687 5288852 87461
+ mean_FusionHeat                1      2072 5289467 87463
+ wtd_std_fie                    1      1856 5289683 87463
+ wtd_mean_atomic_radius         1      1685 5289855 87464
+ wtd_range_atomic_mass          1      1584 5289956 87464
+ wtd_gmean_atomic_mass          1      1546 5289994 87464
+ wtd_mean_atomic_mass           1      1154 5290386 87465
+ mean_ThermalConductivity       1      1013 5290526 87465
+ wtd_range_fie                  1       930 5290610 87466
+ std_FusionHeat                 1       923 5290617 87466
+ entropy_fie                    1       913 5290626 87466
<none>                                     5291540 87466
+ wtd_range_Density              1       624 5290916 87467
+ std_Density                    1       618 5290922 87467
+ wtd_range_ElectronAffinity     1       499 5291041 87467
+ number_of_elements             1       267 5291273 87468
+ entropy_atomic_radius          1       179 5291360 87468
+ wtd_gmean_FusionHeat           1        92 5291448 87468
+ entropy_Valence                1        25 5291514 87468
+ wtd_mean_FusionHeat            1         4 5291536 87468
+ wtd_entropy_Valence            1         1 5291538 87468

Step:  AIC=87351.33
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity

                              Df Sum of Sq     RSS   AIC
+ std_ElectronAffinity         1     39819 5210289 87240
+ mean_fie                     1     24633 5225476 87283
+ gmean_fie                    1     22567 5227542 87289
+ range_Valence                1     19036 5231073 87299
+ gmean_atomic_radius          1     18048 5232060 87302
+ std_ThermalConductivity      1     17203 5232906 87304
+ gmean_Density                1     15272 5234837 87310
+ mean_atomic_radius           1     14426 5235683 87312
+ range_fie                    1     14273 5235836 87313
```

```
+ wtd_range_ThermalConductivity  1     12934 5237175 87317
+ wtd_std_atomic_radius          1     12601 5237508 87318
+ gmean_Valence                  1     12142 5237966 87319
+ std_Valence                    1     11143 5238965 87322
+ entropy_ThermalConductivity    1     11129 5238980 87322
+ wtd_range_atomic_radius        1     10665 5239443 87323
+ mean_Valence                   1     10656 5239452 87323
+ mean_Density                   1     10247 5239861 87324
+ wtd_mean_fie                   1     10211 5239897 87324
+ wtd_gmean_fie                  1      9612 5240496 87326
+ mean_ElectronAffinity          1      8010 5242098 87331
+ wtd_std_Density                1      7816 5242293 87331
+ wtd_std_FusionHeat             1      7356 5242752 87332
+ range_ElectronAffinity         1      7263 5242845 87333
+ entropy_atomic_mass            1      7161 5242948 87333
+ range_FusionHeat               1      6568 5243540 87335
+ wtd_entropy_atomic_radius      1      6403 5243705 87335
+ std_fie                        1      6003 5244106 87336
+ entropy_Density                1      5804 5244304 87337
+ wtd_gmean_Valence              1      5695 5244413 87337
+ wtd_mean_Valence               1      4992 5245116 87339
+ gmean_FusionHeat               1      4807 5245302 87340
+ mean_FusionHeat                1      4473 5245635 87341
+ gmean_atomic_mass              1      3845 5246263 87342
+ std_FusionHeat                 1      3797 5246311 87343
+ wtd_mean_Density               1      3729 5246379 87343
+ wtd_entropy_fie                1      3336 5246773 87344
+ mean_atomic_mass               1      3083 5247025 87345
+ wtd_gmean_Density              1      2960 5247148 87345
+ wtd_range_atomic_mass          1      2339 5247769 87347
+ wtd_gmean_atomic_radius        1      2208 5247900 87347
+ entropy_FusionHeat             1      1914 5248195 87348
+ wtd_std_fie                    1      1788 5248320 87348
+ wtd_range_fie                  1      1751 5248358 87348
+ wtd_range_FusionHeat           1      1624 5248485 87349
+ number_of_elements             1      1570 5248539 87349
+ wtd_entropy_Valence            1      1496 5248612 87349
+ std_atomic_mass                1      1458 5248650 87349
+ wtd_gmean_atomic_mass          1      1076 5249032 87350
+ std_Density                    1      1072 5249036 87350
+ wtd_range_Density              1       929 5249180 87351
+ wtd_mean_atomic_mass           1       870 5249238 87351
<none>                                      5250108 87351
+ wtd_mean_atomic_radius         1       529 5249579 87352
+ mean_ThermalConductivity       1       454 5249654 87352
+ wtd_mean_FusionHeat            1       422 5249686 87352
+ wtd_range_ElectronAffinity     1       378 5249731 87352
+ entropy_fie                    1       300 5249809 87352
```

```
+ entropy_atomic_radius          1       284 5249825 87353
+ entropy_Valence                1        66 5250043 87353
+ wtd_gmean_FusionHeat           1        17 5250091 87353

Step:  AIC=87240.02
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity

                               Df Sum of Sq     RSS   AIC
+ range_ElectronAffinity        1     66651 5143638 87050
+ entropy_atomic_mass           1     27119 5183170 87164
+ wtd_range_ThermalConductivity 1     20739 5189550 87183
+ std_ThermalConductivity       1     19554 5190735 87186
+ entropy_ThermalConductivity   1     18580 5191709 87189
+ wtd_std_atomic_radius         1     18438 5191851 87189
+ mean_ElectronAffinity         1     16294 5193995 87195
+ number_of_elements            1     15701 5194588 87197
+ wtd_range_atomic_radius       1     13744 5196544 87203
+ entropy_Density               1     11255 5199034 87210
+ entropy_atomic_radius         1     10866 5199423 87211
+ range_FusionHeat              1      9188 5201101 87216
+ gmean_fie                     1      9125 5201164 87216
+ mean_fie                      1      8970 5201319 87216
+ gmean_Density                 1      8572 5201717 87218
+ entropy_Valence               1      8077 5202212 87219
+ range_Valence                 1      7676 5202612 87220
+ wtd_entropy_atomic_radius     1      7609 5202680 87220
+ gmean_atomic_radius           1      6840 5203449 87222
+ wtd_std_FusionHeat            1      6360 5203929 87224
+ mean_Density                  1      5957 5204332 87225
+ wtd_entropy_fie               1      5902 5204387 87225
+ std_FusionHeat                1      5787 5204502 87225
+ entropy_fie                   1      5717 5204571 87226
+ mean_atomic_radius            1      5251 5205037 87227
+ gmean_Valence                 1      4625 5205664 87229
+ std_Valence                   1      4540 5205748 87229
+ wtd_mean_fie                  1      4515 5205774 87229
+ wtd_gmean_fie                 1      4396 5205892 87229
+ mean_FusionHeat               1      4018 5206271 87231
+ mean_Valence                  1      3994 5206295 87231
```

```
+ wtd_std_Density                1      3774 5206515 87231
+ entropy_FusionHeat             1      3413 5206876 87232
+ wtd_range_ElectronAffinity     1      3289 5207000 87233
+ wtd_range_atomic_mass          1      3087 5207202 87233
+ gmean_FusionHeat               1      2569 5207720 87235
+ gmean_atomic_mass              1      2408 5207880 87235
+ mean_atomic_mass               1      1453 5208836 87238
+ wtd_entropy_Valence            1      1377 5208912 87238
+ range_fie                      1      1050 5209239 87239
+ wtd_mean_Density               1      1034 5209255 87239
+ std_Density                    1       750 5209538 87240
<none>                                      5210289 87240
+ std_atomic_mass                1       692 5209596 87240
+ mean_ThermalConductivity       1       691 5209598 87240
+ wtd_gmean_Valence              1       570 5209719 87240
+ wtd_range_fie                  1       547 5209742 87240
+ wtd_range_FusionHeat           1       480 5209808 87241
+ wtd_mean_atomic_radius         1       427 5209861 87241
+ wtd_gmean_atomic_mass          1       387 5209902 87241
+ wtd_gmean_Density              1       353 5209936 87241
+ wtd_std_fie                    1       347 5209941 87241
+ wtd_mean_FusionHeat            1       289 5210000 87241
+ wtd_mean_Valence               1       250 5210039 87241
+ wtd_mean_atomic_mass           1       197 5210092 87241
+ wtd_range_Density              1       136 5210153 87242
+ wtd_gmean_atomic_radius        1        19 5210270 87242
+ std_fie                        1        14 5210275 87242
+ wtd_gmean_FusionHeat           1         4 5210285 87242

Step:  AIC=87050.39
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity

                               Df Sum of Sq     RSS   AIC
+ wtd_range_ThermalConductivity  1     34968 5108670 86951
+ entropy_atomic_mass            1     30197 5113441 86965
+ entropy_Density                1     25895 5117743 86977
+ wtd_std_atomic_radius          1     21610 5122028 86990
+ entropy_ThermalConductivity    1     21310 5122327 86991
+ wtd_range_atomic_radius        1     20829 5122809 86992
```

```
+ range_Valence                 1     19074 5124564 86997
+ range_FusionHeat              1     18539 5125099 86999
+ mean_ElectronAffinity         1     18290 5125348 86999
+ mean_fie                      1     15799 5127838 87007
+ entropy_atomic_radius         1     15493 5128145 87007
+ wtd_range_ElectronAffinity    1     14819 5128818 87009
+ gmean_Density                 1     14641 5128997 87010
+ std_FusionHeat                1     13982 5129656 87012
+ std_ThermalConductivity       1     13868 5129770 87012
+ gmean_fie                     1     13154 5130484 87014
+ entropy_Valence               1     12359 5131279 87017
+ wtd_std_FusionHeat            1     11510 5132128 87019
+ range_fie                     1     11245 5132393 87020
+ gmean_atomic_radius           1      9898 5133740 87024
+ gmean_Valence                 1      9501 5134137 87025
+ mean_Density                  1      8456 5135182 87028
+ entropy_fie                   1      8308 5135330 87028
+ wtd_entropy_fie               1      8087 5135551 87029
+ mean_Valence                  1      7479 5136159 87031
+ wtd_std_Density               1      6885 5136752 87032
+ mean_atomic_radius            1      6803 5136835 87033
+ std_Valence                   1      6461 5137177 87034
+ wtd_entropy_atomic_radius     1      6418 5137220 87034
+ wtd_mean_fie                  1      6401 5137237 87034
+ wtd_range_atomic_mass         1      5349 5138289 87037
+ mean_FusionHeat               1      5311 5138327 87037
+ wtd_gmean_fie                 1      5016 5138622 87038
+ number_of_elements            1      4538 5139099 87039
+ gmean_atomic_mass             1      4376 5139262 87040
+ wtd_entropy_Valence           1      3984 5139653 87041
+ wtd_range_fie                 1      3509 5140129 87042
+ entropy_FusionHeat            1      3474 5140164 87042
+ wtd_std_fie                   1      2900 5140738 87044
+ mean_atomic_mass              1      2588 5141049 87045
+ std_fie                       1      2520 5141117 87045
+ wtd_gmean_Density             1      2227 5141410 87046
+ std_atomic_mass               1      2156 5141482 87046
+ wtd_mean_Density              1      1970 5141668 87047
+ gmean_FusionHeat              1      1907 5141730 87047
+ wtd_range_Density             1      1442 5142196 87048
+ wtd_gmean_atomic_mass         1      1062 5142576 87049
+ wtd_gmean_Valence             1       716 5142922 87050
<none>                                     5143638 87050
+ wtd_mean_FusionHeat           1       606 5143032 87051
+ wtd_mean_atomic_mass          1       509 5143129 87051
+ mean_ThermalConductivity      1       469 5143168 87051
+ wtd_gmean_atomic_radius       1       248 5143390 87052
+ wtd_mean_atomic_radius        1       231 5143406 87052
```

```
+ wtd_mean_Valence               1       223 5143414 87052
+ wtd_range_FusionHeat           1        17 5143620 87052
+ wtd_gmean_FusionHeat           1        12 5143626 87052
+ std_Density                    1         4 5143634 87052

Step:  AIC=86950.86
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity

                             Df Sum of Sq     RSS   AIC
+ wtd_std_atomic_radius        1   25432.4 5083238 86879
+ entropy_atomic_mass          1   25397.5 5083273 86879
+ std_ThermalConductivity      1   24917.5 5083753 86880
+ range_Valence                1   23021.3 5085649 86886
+ mean_ElectronAffinity        1   20893.9 5087776 86892
+ entropy_Density              1   19269.4 5089401 86897
+ range_FusionHeat             1   16420.4 5092250 86905
+ mean_fie                     1   15517.0 5093153 86908
+ gmean_Valence                1   14379.1 5094291 86911
+ wtd_range_atomic_radius      1   13001.7 5095668 86915
+ entropy_ThermalConductivity  1   12995.8 5095674 86915
+ gmean_fie                    1   12810.7 5095859 86915
+ gmean_Density                1   12126.0 5096544 86917
+ range_fie                    1   12034.5 5096636 86918
+ std_FusionHeat               1   11932.8 5096737 86918
+ wtd_std_Density              1   11897.7 5096772 86918
+ mean_Valence                 1   11342.5 5097328 86920
+ wtd_std_FusionHeat           1   10596.7 5098073 86922
+ std_Valence                  1    9807.6 5098863 86924
+ entropy_atomic_radius        1    9602.9 5099067 86925
+ gmean_atomic_radius          1    9415.4 5099255 86925
+ entropy_Valence              1    9232.0 5099438 86926
+ wtd_mean_fie                 1    7646.1 5101024 86931
+ mean_Density                 1    7155.8 5101514 86932
+ mean_FusionHeat              1    7030.9 5101639 86932
+ wtd_range_ElectronAffinity   1    6740.3 5101930 86933
+ wtd_entropy_fie              1    6685.5 5101985 86933
+ wtd_entropy_atomic_radius    1    6451.8 5102218 86934
+ mean_atomic_radius           1    6346.9 5102323 86934
```

```
+ number_of_elements           1    6152.0 5102518 86935
+ wtd_gmean_fie                1    5925.6 5102744 86936
+ entropy_fie                  1    4354.1 5104316 86940
+ wtd_gmean_Valence            1    4179.8 5104490 86941
+ gmean_FusionHeat             1    3943.4 5104727 86941
+ gmean_atomic_mass            1    3744.3 5104926 86942
+ wtd_std_fie                  1    3688.7 5104981 86942
+ wtd_mean_Valence             1    2857.4 5105813 86945
+ std_fie                      1    2774.6 5105895 86945
+ wtd_range_atomic_mass        1    2413.5 5106257 86946
+ mean_atomic_mass             1    2088.2 5106582 86947
+ wtd_entropy_Valence          1    2066.5 5106604 86947
+ entropy_FusionHeat           1    1682.4 5106988 86948
+ std_atomic_mass              1    1499.0 5107171 86948
+ wtd_gmean_Density            1    1427.4 5107243 86949
+ wtd_mean_Density             1    1333.1 5107337 86949
+ wtd_mean_FusionHeat          1    1202.9 5107467 86949
<none>                                   5108670 86951
+ wtd_gmean_atomic_radius      1     437.7 5108232 86952
+ wtd_gmean_atomic_mass        1     432.6 5108238 86952
+ wtd_gmean_FusionHeat         1     321.5 5108349 86952
+ mean_ThermalConductivity     1     262.0 5108408 86952
+ wtd_range_FusionHeat         1     202.3 5108468 86952
+ wtd_range_fie                1     187.7 5108482 86952
+ wtd_mean_atomic_radius       1     157.2 5108513 86952
+ wtd_mean_atomic_mass         1      98.3 5108572 86953
+ std_Density                  1      71.4 5108599 86953
+ wtd_range_Density            1      36.7 5108633 86953

Step:  AIC=86878.58
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius

                             Df Sum of Sq     RSS   AIC
+ entropy_atomic_mass          1   26013.4 5057224 86804
+ std_ThermalConductivity      1   25788.0 5057450 86805
+ range_Valence                1   21652.4 5061585 86817
+ gmean_Valence                1   19972.6 5063265 86822
+ mean_ElectronAffinity        1   18135.7 5065102 86827
```

```
+ wtd_range_atomic_radius      1   17872.1 5065366 86828
+ entropy_Density              1   16676.6 5066561 86832
+ mean_Valence                 1   15970.9 5067267 86834
+ wtd_std_FusionHeat           1   15278.5 5067959 86836
+ range_FusionHeat             1   15146.1 5068092 86836
+ entropy_ThermalConductivity  1   13997.7 5069240 86840
+ entropy_Valence              1   13825.4 5069412 86840
+ wtd_std_Density              1   12958.7 5070279 86843
+ entropy_atomic_radius        1   11568.8 5071669 86847
+ std_FusionHeat               1   10600.1 5072638 86850
+ wtd_entropy_fie              1    9988.6 5073249 86851
+ range_fie                    1    9230.6 5074007 86854
+ gmean_Density                1    9030.6 5074207 86854
+ std_Valence                  1    8792.5 5074445 86855
+ mean_fie                     1    8076.7 5075161 86857
+ wtd_entropy_Valence          1    8074.5 5075163 86857
+ mean_FusionHeat              1    7916.3 5075321 86857
+ entropy_fie                  1    6883.1 5076355 86860
+ mean_Density                 1    6417.9 5076820 86862
+ wtd_range_ElectronAffinity   1    6336.2 5076901 86862
+ number_of_elements           1    6271.6 5076966 86862
+ wtd_entropy_atomic_radius    1    6083.4 5077154 86863
+ gmean_fie                    1    5707.2 5077530 86864
+ gmean_FusionHeat             1    5642.8 5077595 86864
+ gmean_atomic_radius          1    4699.8 5078538 86867
+ wtd_gmean_Valence            1    3926.1 5079312 86869
+ wtd_range_atomic_mass        1    3049.1 5080189 86872
+ wtd_mean_Valence             1    2535.0 5080703 86873
+ mean_atomic_radius           1    2488.7 5080749 86873
+ wtd_range_fie                1    2283.1 5080955 86874
+ entropy_FusionHeat           1    2096.5 5081141 86874
+ std_fie                      1    1911.7 5081326 86875
+ wtd_mean_fie                 1    1879.7 5081358 86875
+ wtd_gmean_fie                1    1802.0 5081436 86875
+ wtd_range_FusionHeat         1    1786.8 5081451 86875
+ gmean_atomic_mass            1    1395.6 5081842 86876
+ wtd_range_Density            1     683.3 5082554 86879
<none>                                     5083238 86879
+ wtd_mean_atomic_radius       1     669.1 5082569 86879
+ wtd_mean_Density             1     518.9 5082719 86879
+ std_atomic_mass              1     503.6 5082734 86879
+ mean_atomic_mass             1     443.7 5082794 86879
+ std_Density                  1     306.8 5082931 86880
+ wtd_gmean_Density            1     229.4 5083008 86880
+ wtd_std_fie                  1     209.0 5083029 86880
+ wtd_mean_atomic_mass         1     204.4 5083033 86880
+ wtd_mean_FusionHeat          1     190.0 5083048 86880
+ wtd_gmean_atomic_radius      1     170.0 5083068 86880
```

```
+ wtd_gmean_FusionHeat         1     152.8 5083085 86880
+ wtd_gmean_atomic_mass        1      58.1 5083180 86880
+ mean_ThermalConductivity     1       6.0 5083232 86881

Step:  AIC=86804.21
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass

                             Df Sum of Sq     RSS   AIC
+ wtd_std_FusionHeat           1   24484.6 5032740 86734
+ range_FusionHeat             1   24394.6 5032830 86734
+ range_Valence                1   20433.0 5036791 86746
+ std_ThermalConductivity      1   20394.4 5036830 86746
+ wtd_entropy_fie              1   20373.7 5036851 86746
+ std_FusionHeat               1   18840.0 5038384 86751
+ gmean_Valence                1   16980.8 5040243 86756
+ wtd_std_Density              1   16726.3 5040498 86757
+ mean_Valence                 1   13891.7 5043333 86765
+ mean_FusionHeat              1   13530.6 5043694 86766
+ mean_ElectronAffinity        1   11084.3 5046140 86774
+ range_fie                    1    9696.0 5047528 86778
+ wtd_range_ElectronAffinity   1    9081.5 5048143 86779
+ gmean_FusionHeat             1    8543.8 5048681 86781
+ wtd_range_atomic_radius      1    8291.6 5048933 86782
+ entropy_ThermalConductivity  1    8157.6 5049067 86782
+ gmean_Density                1    8143.3 5049081 86782
+ std_Valence                  1    6912.8 5050311 86786
+ mean_fie                     1    6430.2 5050794 86787
+ mean_Density                 1    6061.4 5051163 86788
+ std_atomic_mass              1    5376.4 5051848 86790
+ wtd_entropy_atomic_radius    1    4973.1 5052251 86792
+ gmean_fie                    1    4346.8 5052878 86793
+ wtd_entropy_Valence          1    4304.9 5052919 86794
+ wtd_range_fie                1    3662.4 5053562 86795
+ wtd_mean_atomic_radius       1    3122.3 5054102 86797
+ wtd_gmean_Valence            1    2722.6 5054502 86798
+ wtd_mean_atomic_mass         1    2453.3 5054771 86799
+ gmean_atomic_radius          1    2288.5 5054936 86799
+ wtd_gmean_atomic_mass        1    2230.4 5054994 86800
```

```
+ wtd_gmean_atomic_radius      1    2035.3 5055189 86800
+ std_fie                      1    2011.1 5055213 86800
+ wtd_mean_Valence             1    1709.5 5055515 86801
+ wtd_mean_FusionHeat          1    1605.4 5055619 86801
+ entropy_Density              1    1232.5 5055992 86803
+ mean_atomic_radius           1    1001.2 5056223 86803
+ entropy_FusionHeat           1     870.5 5056354 86804
+ mean_ThermalConductivity     1     680.4 5056544 86804
<none>                                   5057224 86804
+ entropy_Valence              1     608.8 5056616 86804
+ number_of_elements           1     607.9 5056616 86804
+ std_Density                  1     401.9 5056822 86805
+ wtd_std_fie                  1     326.6 5056898 86805
+ wtd_range_FusionHeat         1     316.4 5056908 86805
+ entropy_fie                  1     278.9 5056945 86805
+ wtd_mean_fie                 1     204.3 5057020 86806
+ wtd_gmean_fie                1     172.1 5057052 86806
+ wtd_mean_Density             1     143.0 5057081 86806
+ wtd_range_atomic_mass        1      81.7 5057143 86806
+ wtd_range_Density            1      76.4 5057148 86806
+ wtd_gmean_FusionHeat         1      61.7 5057163 86806
+ wtd_gmean_Density            1      16.8 5057208 86806
+ entropy_atomic_radius        1      13.5 5057211 86806
+ gmean_atomic_mass            1       7.3 5057217 86806
+ mean_atomic_mass             1       1.6 5057223 86806

Step:  AIC=86733.98
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat

                              Df Sum of Sq     RSS   AIC
+ wtd_entropy_fie              1   23556.5 5009183 86666
+ range_Valence                1   20612.6 5012127 86675
+ wtd_range_FusionHeat         1   17449.3 5015290 86684
+ wtd_range_ElectronAffinity   1   13639.4 5019100 86696
+ wtd_range_atomic_radius      1   12556.9 5020183 86699
+ std_ThermalConductivity      1   12348.5 5020391 86699
```

```
+ gmean_Valence                1   11221.2 5021519 86703
+ wtd_entropy_atomic_radius    1   10941.2 5021798 86704
+ mean_fie                     1   10102.9 5022637 86706
+ wtd_std_Density              1    9495.1 5023245 86708
+ mean_ElectronAffinity        1    9330.5 5023409 86708
+ mean_Valence                 1    9131.8 5023608 86709
+ mean_Density                 1    8993.8 5023746 86709
+ gmean_fie                    1    8773.5 5023966 86710
+ gmean_Density                1    8348.1 5024392 86711
+ gmean_atomic_radius          1    7599.9 5025140 86713
+ std_Valence                  1    7539.6 5025200 86714
+ entropy_fie                  1    7313.9 5025426 86714
+ range_fie                    1    6366.7 5026373 86717
+ std_atomic_mass              1    6142.7 5026597 86718
+ mean_atomic_radius           1    5126.9 5027613 86721
+ wtd_mean_FusionHeat          1    5057.5 5027682 86721
+ wtd_gmean_FusionHeat         1    4167.9 5028572 86724
+ entropy_atomic_radius        1    3837.7 5028902 86725
+ wtd_range_fie                1    2801.7 5029938 86728
+ entropy_ThermalConductivity  1    2126.4 5030613 86730
+ wtd_gmean_fie                1    1996.8 5030743 86730
+ gmean_atomic_mass            1    1612.2 5031128 86731
+ entropy_Valence              1    1524.6 5031215 86731
+ wtd_mean_fie                 1    1488.7 5031251 86732
+ wtd_gmean_Valence            1    1464.9 5031275 86732
+ mean_ThermalConductivity     1    1458.0 5031282 86732
+ wtd_std_fie                  1    1420.4 5031319 86732
+ entropy_Density              1    1310.0 5031430 86732
+ range_FusionHeat             1    1191.8 5031548 86732
+ mean_atomic_mass             1    1068.6 5031671 86733
+ wtd_mean_Valence             1     898.2 5031842 86733
+ wtd_range_atomic_mass        1     891.7 5031848 86733
+ wtd_entropy_Valence          1     885.9 5031854 86733
<none>                                     5032740 86734
+ std_fie                      1     674.3 5032065 86734
+ gmean_FusionHeat             1     581.9 5032158 86734
+ wtd_mean_Density             1     568.4 5032171 86734
+ std_FusionHeat               1     376.0 5032364 86735
+ number_of_elements           1     248.4 5032491 86735
+ std_Density                  1     230.4 5032509 86735
+ mean_FusionHeat              1     108.8 5032631 86736
+ wtd_mean_atomic_mass         1     105.1 5032635 86736
+ wtd_gmean_Density            1     102.4 5032637 86736
+ wtd_gmean_atomic_radius      1      34.9 5032705 86736
+ wtd_gmean_atomic_mass        1      21.6 5032718 86736
+ wtd_mean_atomic_radius       1      17.8 5032722 86736
+ wtd_range_Density            1       8.3 5032731 86736
+ entropy_FusionHeat           1       4.1 5032736 86736
```

```
Step:  AIC=86666.15
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie

                             Df Sum of Sq     RSS   AIC
+ range_Valence               1   26122.4 4983061 86590
+ wtd_entropy_Valence         1   22654.5 4986529 86601
+ wtd_range_FusionHeat        1   21840.2 4987343 86603
+ wtd_range_ElectronAffinity  1   16307.0 4992876 86620
+ std_Valence                 1   12804.6 4996379 86630
+ std_ThermalConductivity     1   11208.8 4997974 86635
+ wtd_std_Density             1   10876.7 4998307 86636
+ wtd_range_atomic_radius     1    9426.1 4999757 86640
+ gmean_Valence               1    8497.8 5000685 86643
+ mean_ElectronAffinity       1    6750.1 5002433 86648
+ wtd_mean_FusionHeat         1    6412.8 5002770 86649
+ mean_Valence                1    6347.4 5002836 86649
+ wtd_gmean_FusionHeat        1    5429.1 5003754 86652
+ mean_Density                1    5213.1 5003970 86653
+ std_atomic_mass             1    4520.4 5004663 86655
+ gmean_Density               1    4044.9 5005138 86656
+ entropy_Density             1    3800.7 5005383 86657
+ wtd_gmean_Valence           1    3511.5 5005672 86658
+ range_fie                   1    3454.9 5005728 86658
+ wtd_gmean_fie               1    3364.1 5005819 86658
+ wtd_mean_fie                1    2991.9 5006191 86659
+ wtd_mean_Valence            1    2836.0 5006347 86660
+ wtd_entropy_atomic_radius   1    2771.2 5006412 86660
+ mean_fie                    1    2490.0 5006693 86661
+ wtd_range_fie               1    2457.9 5006725 86661
+ gmean_fie                   1    1843.5 5007340 86663
+ gmean_atomic_radius         1    1390.4 5007793 86664
+ wtd_mean_Density            1    1384.0 5007799 86664
+ entropy_fie                 1    1235.4 5007948 86664
+ wtd_range_atomic_mass       1    1158.2 5008025 86665
+ wtd_std_fie                 1    1067.7 5008116 86665
```

```
+ range_FusionHeat             1     963.8 5008219 86665
+ wtd_gmean_atomic_radius      1     676.9 5008506 86666
<none>                                     5009183 86666
+ std_FusionHeat               1     600.1 5008583 86666
+ entropy_atomic_radius        1     426.6 5008757 86667
+ mean_atomic_radius           1     403.5 5008780 86667
+ entropy_FusionHeat           1     309.2 5008874 86667
+ entropy_ThermalConductivity  1     272.1 5008911 86667
+ wtd_range_Density            1     256.8 5008926 86667
+ entropy_Valence              1     211.9 5008971 86668
+ wtd_mean_atomic_radius       1     180.3 5009003 86668
+ mean_ThermalConductivity     1     174.8 5009008 86668
+ gmean_atomic_mass            1     117.2 5009066 86668
+ gmean_FusionHeat             1      90.9 5009092 86668
+ wtd_gmean_Density            1      77.2 5009106 86668
+ std_Density                  1      61.3 5009122 86668
+ std_fie                      1      46.3 5009137 86668
+ mean_FusionHeat              1      26.6 5009157 86668
+ mean_atomic_mass             1      10.6 5009173 86668
+ number_of_elements           1       7.6 5009176 86668
+ wtd_mean_atomic_mass         1       2.6 5009181 86668
+ wtd_gmean_atomic_mass        1       1.6 5009182 86668

Step:  AIC=86590.32
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence

                              Df Sum of Sq     RSS   AIC
+ wtd_entropy_Valence          1   29424.2 4953637 86504
+ wtd_range_FusionHeat         1   23811.9 4959249 86521
+ wtd_range_ElectronAffinity   1   17032.2 4966029 86541
+ std_ThermalConductivity      1   12954.2 4970107 86554
+ wtd_range_atomic_radius      1    8794.3 4974267 86566
+ mean_Valence                 1    8341.8 4974719 86567
+ std_Valence                  1    7851.9 4975209 86569
+ gmean_Valence                1    7521.8 4975539 86570
+ wtd_mean_FusionHeat          1    7430.3 4975631 86570
```

```
+ wtd_gmean_FusionHeat         1    6494.9 4976566 86573
+ wtd_std_Density              1    5694.1 4977367 86575
+ range_FusionHeat             1    5183.1 4977878 86577
+ mean_ElectronAffinity        1    4936.8 4978124 86578
+ std_atomic_mass              1    4665.5 4978395 86578
+ mean_Density                 1    4558.1 4978503 86579
+ entropy_Density              1    4488.7 4978572 86579
+ wtd_gmean_Valence            1    3610.5 4979450 86582
+ wtd_entropy_atomic_radius    1    3303.4 4979758 86582
+ wtd_gmean_fie                1    3290.8 4979770 86582
+ entropy_FusionHeat           1    3001.4 4980059 86583
+ wtd_mean_fie                 1    2884.9 4980176 86584
+ gmean_Density                1    2883.3 4980178 86584
+ wtd_mean_Valence             1    2806.3 4980255 86584
+ mean_fie                     1    2171.9 4980889 86586
+ range_fie                    1    1980.4 4981081 86586
+ wtd_range_fie                1    1965.3 4981096 86586
+ gmean_fie                    1    1683.1 4981378 86587
+ entropy_Valence              1    1680.8 4981380 86587
+ gmean_atomic_radius          1    1309.3 4981752 86588
+ wtd_std_fie                  1    1229.9 4981831 86589
+ wtd_range_atomic_mass        1    1124.5 4981936 86589
+ wtd_mean_Density             1     831.1 4982230 86590
+ entropy_fie                  1     793.7 4982267 86590
<none>                                    4983061 86590
+ wtd_gmean_atomic_radius      1     595.8 4982465 86591
+ number_of_elements           1     483.0 4982578 86591
+ mean_atomic_radius           1     400.8 4982660 86591
+ std_FusionHeat               1     189.8 4982871 86592
+ wtd_mean_atomic_radius       1     167.5 4982893 86592
+ entropy_atomic_radius        1     140.5 4982920 86592
+ gmean_atomic_mass            1      58.5 4983002 86592
+ std_Density                  1      37.4 4983024 86592
+ entropy_ThermalConductivity  1      19.8 4983041 86592
+ mean_ThermalConductivity     1      19.3 4983042 86592
+ wtd_range_Density            1      18.8 4983042 86592
+ wtd_gmean_atomic_mass        1      14.1 4983047 86592
+ mean_FusionHeat              1      10.7 4983050 86592
+ wtd_gmean_Density            1       5.5 4983055 86592
+ std_fie                      1       0.6 4983060 86592
+ wtd_mean_atomic_mass         1       0.4 4983061 86592
+ mean_atomic_mass             1       0.1 4983061 86592
+ gmean_FusionHeat             1       0.0 4983061 86592

Step:  AIC=86504.18
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
```

```
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence

                              Df Sum of Sq     RSS   AIC
+ wtd_range_FusionHeat         1   21995.9 4931641 86440
+ wtd_range_fie                1   16510.5 4937126 86456
+ std_ThermalConductivity      1   13569.9 4940067 86465
+ wtd_entropy_atomic_radius    1    8043.6 4945593 86482
+ wtd_range_ElectronAffinity   1    7770.0 4945867 86483
+ wtd_gmean_fie                1    7516.1 4946121 86484
+ wtd_mean_fie                 1    7513.0 4946124 86484
+ range_FusionHeat             1    6667.8 4946969 86486
+ entropy_Valence              1    6623.5 4947013 86486
+ wtd_mean_FusionHeat          1    5699.4 4947937 86489
+ mean_ElectronAffinity        1    5420.4 4948216 86490
+ std_atomic_mass              1    5235.7 4948401 86490
+ wtd_gmean_FusionHeat         1    5154.7 4948482 86491
+ wtd_std_Density              1    4627.2 4949009 86492
+ std_Valence                  1    3843.1 4949794 86495
+ range_fie                    1    3603.4 4950033 86495
+ mean_fie                     1    3546.9 4950090 86496
+ gmean_fie                    1    2792.5 4950844 86498
+ gmean_atomic_radius          1    2773.2 4950863 86498
+ entropy_FusionHeat           1    2758.5 4950878 86498
+ mean_Density                 1    2565.9 4951071 86498
+ wtd_range_atomic_radius      1    2461.8 4951175 86499
+ entropy_fie                  1    2306.0 4951331 86499
+ gmean_Density                1    2300.2 4951336 86499
+ wtd_gmean_Valence            1    2273.6 4951363 86499
+ wtd_range_Density            1    2222.5 4951414 86499
+ entropy_Density              1    2181.9 4951455 86500
+ wtd_mean_Valence             1    2128.7 4951508 86500
+ entropy_ThermalConductivity  1    1565.4 4952071 86501
+ mean_Valence                 1    1559.9 4952077 86501
+ wtd_gmean_atomic_radius      1    1199.8 4952437 86503
+ gmean_Valence                1    1066.4 4952570 86503
+ mean_atomic_radius           1     949.3 4952687 86503
+ std_FusionHeat               1     790.0 4952847 86504
+ entropy_atomic_radius        1     712.8 4952924 86504
<none>                                   4953637 86504
```

```
+ std_Density                  1     399.6 4953237 86505
+ wtd_mean_atomic_radius       1     326.6 4953310 86505
+ std_fie                      1     234.4 4953402 86505
+ wtd_mean_Density             1     143.2 4953493 86506
+ mean_FusionHeat              1     134.4 4953502 86506
+ number_of_elements           1     131.1 4953506 86506
+ gmean_FusionHeat             1     119.6 4953517 86506
+ gmean_atomic_mass            1     116.4 4953520 86506
+ mean_ThermalConductivity     1     115.2 4953521 86506
+ wtd_gmean_Density            1      60.9 4953576 86506
+ wtd_std_fie                  1      47.2 4953589 86506
+ wtd_range_atomic_mass        1      42.5 4953594 86506
+ wtd_gmean_atomic_mass        1      37.9 4953599 86506
+ mean_atomic_mass             1       2.1 4953635 86506
+ wtd_mean_atomic_mass         1       0.0 4953637 86506

Step:  AIC=86439.94
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat

                              Df Sum of Sq     RSS   AIC
+ std_ThermalConductivity      1   18724.7 4912916 86385
+ wtd_range_fie                1   12244.5 4919396 86405
+ range_FusionHeat             1    9604.7 4922036 86413
+ wtd_entropy_atomic_radius    1    8081.9 4923559 86418
+ wtd_range_ElectronAffinity   1    7033.8 4924607 86421
+ entropy_Valence              1    6015.7 4925625 86424
+ std_FusionHeat               1    5733.6 4925907 86425
+ std_Valence                  1    5141.8 4926499 86426
+ mean_ElectronAffinity        1    4555.5 4927085 86428
+ wtd_gmean_Valence            1    4527.6 4927113 86428
+ wtd_mean_Valence             1    4167.3 4927474 86429
+ wtd_mean_fie                 1    4121.7 4927519 86429
+ wtd_gmean_fie                1    4020.8 4927620 86430
+ wtd_std_Density              1    3915.1 4927726 86430
+ wtd_mean_FusionHeat          1    3824.8 4927816 86430
```

```
+ wtd_range_Density            1    3792.2 4927849 86430
+ entropy_ThermalConductivity  1    3678.8 4927962 86431
+ mean_Valence                 1    3630.5 4928010 86431
+ range_fie                    1    3125.7 4928515 86433
+ gmean_Valence                1    2953.6 4928687 86433
+ gmean_atomic_radius          1    2878.0 4928763 86433
+ mean_Density                 1    2723.6 4928917 86434
+ mean_FusionHeat              1    2665.4 4928975 86434
+ wtd_gmean_FusionHeat         1    2538.1 4929103 86434
+ std_atomic_mass              1    2430.5 4929210 86435
+ gmean_Density                1    2427.9 4929213 86435
+ mean_fie                     1    2346.3 4929294 86435
+ gmean_fie                    1    1840.4 4929800 86436
+ entropy_fie                  1    1800.3 4929840 86437
+ wtd_range_atomic_radius      1    1657.5 4929983 86437
+ std_Density                  1    1364.7 4930276 86438
+ entropy_Density              1    1125.6 4930515 86439
+ mean_atomic_radius           1    1121.6 4930519 86439
+ gmean_FusionHeat             1     930.9 4930710 86439
+ number_of_elements           1     906.7 4930734 86439
+ entropy_FusionHeat           1     816.8 4930824 86439
+ wtd_range_atomic_mass        1     759.7 4930881 86440
+ wtd_gmean_atomic_radius      1     681.1 4930960 86440
<none>                                   4931641 86440
+ entropy_atomic_radius        1     457.5 4931183 86441
+ wtd_mean_atomic_mass         1     245.9 4931395 86441
+ mean_atomic_mass             1     230.2 4931411 86441
+ wtd_gmean_Density            1     161.0 4931480 86441
+ wtd_gmean_atomic_mass        1     123.0 4931518 86442
+ wtd_mean_Density             1     100.6 4931540 86442
+ std_fie                      1     100.5 4931540 86442
+ wtd_mean_atomic_radius       1      95.3 4931545 86442
+ wtd_std_fie                  1      67.1 4931574 86442
+ gmean_atomic_mass            1      24.1 4931617 86442
+ mean_ThermalConductivity     1       1.0 4931640 86442

Step:  AIC=86385.32
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
```

```
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity

                              Df Sum of Sq     RSS   AIC
+ wtd_range_ElectronAffinity   1   12135.5 4900781 86351
+ entropy_Valence              1    9343.6 4903573 86359
+ wtd_range_fie                1    8375.3 4904541 86362
+ wtd_entropy_atomic_radius    1    8040.8 4904875 86363
+ range_FusionHeat             1    6095.7 4906820 86369
+ std_Valence                  1    5182.6 4907733 86372
+ mean_ElectronAffinity        1    5101.4 4907815 86372
+ entropy_fie                  1    4335.9 4908580 86374
+ mean_ThermalConductivity     1    4087.2 4908829 86375
+ std_atomic_mass              1    3714.3 4909202 86376
+ wtd_range_Density            1    3635.6 4909280 86376
+ wtd_gmean_Valence            1    3346.4 4909570 86377
+ std_FusionHeat               1    3070.7 4909845 86378
+ wtd_gmean_fie                1    3058.8 4909857 86378
+ wtd_std_Density              1    3029.9 4909886 86378
+ wtd_mean_Valence             1    3023.5 4909893 86378
+ wtd_mean_fie                 1    3023.0 4909893 86378
+ wtd_mean_FusionHeat          1    2939.8 4909976 86378
+ range_fie                    1    2899.0 4910017 86379
+ mean_Density                 1    2546.3 4910370 86380
+ entropy_atomic_radius        1    2253.6 4910663 86380
+ gmean_Density                1    2250.2 4910666 86381
+ gmean_atomic_radius          1    2241.9 4910674 86381
+ mean_Valence                 1    2116.0 4910800 86381
+ mean_fie                     1    1778.4 4911138 86382
+ wtd_gmean_FusionHeat         1    1764.8 4911151 86382
+ wtd_range_atomic_radius      1    1750.3 4911166 86382
+ number_of_elements           1    1740.4 4911176 86382
+ gmean_Valence                1    1638.7 4911277 86382
+ std_Density                  1    1572.1 4911344 86383
+ gmean_fie                    1    1450.4 4911466 86383
+ entropy_Density              1    1421.1 4911495 86383
+ entropy_FusionHeat           1    1291.7 4911624 86383
+ mean_FusionHeat              1    1226.7 4911689 86384
+ mean_atomic_radius           1     844.5 4912072 86385
<none>                                    4912916 86385
+ wtd_range_atomic_mass        1     606.3 4912310 86385
+ wtd_mean_atomic_mass         1     457.2 4912459 86386
+ gmean_FusionHeat             1     412.6 4912503 86386
+ wtd_gmean_atomic_mass        1     283.5 4912633 86386
+ wtd_gmean_Density            1     277.6 4912638 86386
+ wtd_std_fie                  1     173.8 4912742 86387
+ mean_atomic_mass             1     161.6 4912754 86387
```

```
+ wtd_gmean_atomic_radius      1     128.0 4912788 86387
+ entropy_ThermalConductivity  1      51.9 4912864 86387
+ wtd_mean_Density             1      17.2 4912899 86387
+ wtd_mean_atomic_radius       1      13.8 4912902 86387
+ gmean_atomic_mass            1       7.1 4912909 86387
+ std_fie                      1       6.3 4912910 86387

Step:  AIC=86350.51
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity

                            Df Sum of Sq     RSS   AIC
+ wtd_range_fie              1   15448.1 4885332 86306
+ wtd_entropy_atomic_radius  1    8203.8 4892577 86328
+ wtd_mean_FusionHeat        1    6822.9 4893958 86332
+ mean_ElectronAffinity      1    6426.4 4894354 86333
+ entropy_Valence            1    5320.7 4895460 86336
+ range_FusionHeat           1    5248.9 4895532 86337
+ wtd_gmean_Valence          1    5073.6 4895707 86337
+ wtd_gmean_FusionHeat       1    5049.0 4895732 86337
+ wtd_mean_Valence           1    4711.7 4896069 86338
+ std_Valence                1    4561.2 4896219 86339
+ wtd_range_Density          1    4179.1 4896601 86340
+ range_fie                  1    3839.2 4896941 86341
+ std_atomic_mass            1    3578.9 4897202 86342
+ mean_Valence               1    3521.2 4897259 86342
+ mean_FusionHeat            1    3280.5 4897500 86343
+ wtd_std_Density            1    3112.2 4897668 86343
+ gmean_Valence              1    3020.8 4897760 86343
+ wtd_mean_fie               1    2947.1 4897833 86344
+ wtd_range_atomic_radius    1    2924.5 4897856 86344
+ wtd_gmean_fie              1    2899.3 4897881 86344
+ mean_ThermalConductivity   1    2449.3 4898331 86345
+ gmean_Density              1    2443.9 4898337 86345
+ mean_Density               1    2371.2 4898409 86345
+ gmean_FusionHeat           1    2325.5 4898455 86345
```

```
+ gmean_atomic_radius          1    2167.0 4898614 86346
+ entropy_fie                  1    2027.0 4898754 86346
+ std_FusionHeat               1    1970.6 4898810 86347
+ std_Density                  1    1664.3 4899116 86347
+ mean_fie                     1    1428.8 4899352 86348
+ wtd_range_atomic_mass        1    1322.7 4899458 86348
+ gmean_fie                    1     966.4 4899814 86350
+ wtd_mean_atomic_mass         1     851.4 4899929 86350
+ mean_atomic_radius           1     752.3 4900028 86350
+ entropy_atomic_radius        1     740.8 4900040 86350
+ wtd_gmean_atomic_mass        1     683.9 4900097 86350
<none>                                     4900781 86351
+ entropy_Density              1     464.0 4900317 86351
+ mean_atomic_mass             1     360.3 4900420 86351
+ number_of_elements           1     306.7 4900474 86352
+ wtd_gmean_Density            1     248.9 4900532 86352
+ std_fie                      1     181.4 4900599 86352
+ entropy_FusionHeat           1     119.9 4900661 86352
+ gmean_atomic_mass            1     112.4 4900668 86352
+ entropy_ThermalConductivity  1      89.5 4900691 86352
+ wtd_gmean_atomic_radius      1      78.0 4900703 86352
+ wtd_std_fie                  1      74.3 4900706 86352
+ wtd_mean_atomic_radius       1      32.7 4900748 86352
+ wtd_mean_Density             1      22.2 4900758 86352

Step:  AIC=86305.52
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie

                             Df Sum of Sq     RSS   AIC
+ mean_ElectronAffinity       1    9130.9 4876202 86280
+ wtd_range_Density           1    7643.7 4877689 86284
+ mean_ThermalConductivity    1    6895.5 4878437 86286
+ range_FusionHeat            1    6465.9 4878867 86288
```

```
+ wtd_mean_atomic_radius       1    6118.1 4879214 86289
+ wtd_entropy_atomic_radius    1    5182.1 4880150 86292
+ wtd_gmean_atomic_radius      1    4116.7 4881216 86295
+ std_atomic_mass              1    4111.9 4881221 86295
+ wtd_mean_atomic_mass         1    3919.4 4881413 86296
+ wtd_mean_FusionHeat          1    3783.3 4881549 86296
+ std_Valence                  1    3620.5 4881712 86296
+ wtd_gmean_atomic_mass        1    3576.5 4881756 86297
+ wtd_std_fie                  1    3288.9 4882044 86297
+ wtd_range_atomic_radius      1    3227.5 4882105 86298
+ std_FusionHeat               1    3169.8 4882163 86298
+ wtd_gmean_Density            1    2836.3 4882496 86299
+ mean_atomic_mass             1    2462.1 4882870 86300
+ wtd_gmean_FusionHeat         1    2287.6 4883045 86301
+ mean_FusionHeat              1    2007.5 4883325 86301
+ gmean_atomic_mass            1    1960.2 4883372 86302
+ entropy_Density              1    1670.6 4883662 86302
+ std_Density                  1    1454.4 4883878 86303
+ std_fie                      1    1313.1 4884019 86304
+ wtd_range_atomic_mass        1    1279.0 4884053 86304
+ wtd_std_Density              1    1211.1 4884121 86304
+ wtd_mean_Density             1     951.1 4884381 86305
+ entropy_Valence              1     904.7 4884428 86305
+ gmean_FusionHeat             1     881.2 4884451 86305
+ mean_Density                 1     862.8 4884470 86305
+ entropy_ThermalConductivity  1     741.0 4884591 86305
<none>                                   4885332 86306
+ entropy_atomic_radius        1     642.2 4884690 86306
+ mean_atomic_radius           1     599.6 4884733 86306
+ entropy_FusionHeat           1     575.3 4884757 86306
+ gmean_fie                    1     476.1 4884856 86306
+ mean_fie                     1     421.4 4884911 86306
+ gmean_Density                1     378.7 4884954 86306
+ wtd_gmean_Valence            1     374.1 4884958 86306
+ wtd_mean_Valence             1     331.3 4885001 86307
+ range_fie                    1     272.0 4885060 86307
+ mean_Valence                 1     261.3 4885071 86307
+ wtd_mean_fie                 1     187.2 4885145 86307
+ wtd_gmean_fie                1      96.9 4885236 86307
+ entropy_fie                  1      96.7 4885236 86307
+ gmean_Valence                1      78.3 4885254 86307
+ gmean_atomic_radius          1      51.1 4885281 86307
+ number_of_elements           1       7.0 4885325 86307

Step:  AIC=86279.67
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
```

```
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity

                            Df Sum of Sq     RSS   AIC
+ wtd_range_Density          1    6370.3 4869831 86262
+ wtd_mean_atomic_radius     1    6084.2 4870117 86263
+ range_FusionHeat           1    5104.2 4871097 86266
+ mean_ThermalConductivity   1    4576.4 4871625 86268
+ std_atomic_mass            1    4470.9 4871731 86268
+ wtd_gmean_atomic_radius    1    4290.4 4871911 86269
+ wtd_std_fie                1    4255.7 4871946 86269
+ std_Valence                1    3242.2 4872959 86272
+ wtd_mean_FusionHeat        1    3238.4 4872963 86272
+ wtd_entropy_atomic_radius  1    3113.0 4873089 86272
+ wtd_mean_atomic_mass       1    2874.0 4873328 86273
+ wtd_gmean_atomic_mass      1    2694.2 4873507 86273
+ wtd_gmean_Density          1    2665.6 4873536 86274
+ std_fie                    1    2419.7 4873782 86274
+ std_FusionHeat             1    2376.3 4873825 86274
+ wtd_range_atomic_radius    1    2282.8 4873919 86275
+ mean_atomic_mass           1    1950.9 4874251 86276
+ entropy_Density            1    1732.3 4874469 86276
+ wtd_gmean_FusionHeat       1    1687.9 4874514 86277
+ std_Density                1    1666.5 4874535 86277
+ gmean_atomic_mass          1    1569.5 4874632 86277
+ wtd_std_Density            1    1564.3 4874637 86277
+ mean_FusionHeat            1    1210.1 4874991 86278
+ entropy_Valence            1     998.1 4875203 86279
+ entropy_FusionHeat         1     891.3 4875310 86279
+ mean_Density               1     802.5 4875399 86279
+ wtd_mean_Density           1     669.1 4875532 86280
<none>                                   4876202 86280
+ wtd_range_atomic_mass      1     557.2 4875644 86280
+ entropy_atomic_radius      1     514.8 4875687 86280
+ gmean_FusionHeat           1     405.4 4875796 86280
+ gmean_Density              1     314.7 4875887 86281
+ mean_atomic_radius         1     280.6 4875921 86281
```

```
+ entropy_ThermalConductivity  1     259.6 4875942 86281
+ wtd_mean_fie                 1     225.5 4875976 86281
+ wtd_gmean_Valence            1     164.9 4876037 86281
+ wtd_mean_Valence             1     148.0 4876054 86281
+ wtd_gmean_fie                1     109.9 4876092 86281
+ number_of_elements           1     108.0 4876094 86281
+ mean_fie                     1      62.4 4876139 86281
+ gmean_fie                    1      45.3 4876156 86282
+ entropy_fie                  1      37.3 4876164 86282
+ mean_Valence                 1      13.4 4876188 86282
+ gmean_Valence                1      11.6 4876190 86282
+ range_fie                    1       1.0 4876201 86282
+ gmean_atomic_radius          1       0.7 4876201 86282

Step:  AIC=86262.22
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density

                             Df Sum of Sq     RSS   AIC
+ std_atomic_mass             1    5574.3 4864257 86247
+ mean_Density                1    4707.5 4865124 86250
+ range_FusionHeat            1    4664.7 4865167 86250
+ wtd_std_fie                 1    4129.3 4865702 86252
+ wtd_mean_atomic_radius      1    3715.6 4866116 86253
+ wtd_mean_FusionHeat         1    3691.9 4866139 86253
+ mean_ThermalConductivity    1    3454.1 4866377 86254
+ std_Valence                 1    3115.4 4866716 86255
+ wtd_range_atomic_radius     1    2726.7 4867105 86256
+ gmean_Density               1    2640.4 4867191 86256
+ wtd_std_Density             1    2621.9 4867209 86256
+ std_fie                     1    2412.6 4867419 86257
+ wtd_gmean_atomic_radius     1    2340.1 4867491 86257
+ wtd_entropy_atomic_radius   1    2246.8 4867585 86257
+ entropy_Valence             1    2143.1 4867688 86258
```

```
+ wtd_range_atomic_mass        1    1972.3 4867859 86258
+ wtd_gmean_FusionHeat         1    1958.6 4867873 86258
+ std_FusionHeat               1    1829.9 4868001 86259
+ wtd_mean_Density             1    1609.6 4868222 86259
+ mean_FusionHeat              1    1236.7 4868595 86260
+ std_Density                  1    1035.8 4868795 86261
+ entropy_FusionHeat           1     897.1 4868934 86261
<none>                                   4869831 86262
+ entropy_Density              1     637.9 4869193 86262
+ wtd_mean_fie                 1     549.3 4869282 86263
+ gmean_FusionHeat             1     487.9 4869343 86263
+ wtd_gmean_fie                1     368.8 4869463 86263
+ wtd_mean_Valence             1     308.4 4869523 86263
+ wtd_gmean_Valence            1     308.1 4869523 86263
+ mean_atomic_mass             1     200.3 4869631 86264
+ gmean_atomic_radius          1     183.9 4869647 86264
+ entropy_ThermalConductivity  1     177.7 4869654 86264
+ wtd_mean_atomic_mass         1     150.0 4869681 86264
+ wtd_gmean_atomic_mass        1     142.4 4869689 86264
+ mean_fie                     1     117.4 4869714 86264
+ gmean_atomic_mass            1     108.7 4869723 86264
+ gmean_fie                    1      93.6 4869738 86264
+ entropy_atomic_radius        1      76.8 4869754 86264
+ entropy_fie                  1      67.2 4869764 86264
+ gmean_Valence                1      30.4 4869801 86264
+ mean_atomic_radius           1       4.5 4869827 86264
+ number_of_elements           1       4.2 4869827 86264
+ mean_Valence                 1       3.2 4869828 86264
+ range_fie                    1       0.6 4869831 86264
+ wtd_gmean_Density            1       0.2 4869831 86264

Step:  AIC=86247.17
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
```

```
    std_atomic_mass

                              Df Sum of Sq     RSS   AIC
+ mean_Density                 1    4726.7 4859530 86235
+ mean_ThermalConductivity     1    4447.2 4859810 86236
+ wtd_std_Density              1    4350.0 4859907 86236
+ wtd_std_fie                  1    4255.9 4860001 86236
+ range_FusionHeat             1    4042.8 4860214 86237
+ entropy_Valence              1    4041.7 4860215 86237
+ wtd_mean_atomic_radius       1    3987.1 4860270 86237
+ wtd_mean_FusionHeat          1    3370.4 4860887 86239
+ gmean_Density                1    2613.6 4861643 86241
+ wtd_gmean_atomic_radius      1    2598.1 4861659 86241
+ std_fie                      1    2432.6 4861824 86242
+ wtd_mean_Density             1    2036.8 4862220 86243
+ std_Valence                  1    1982.0 4862275 86243
+ std_Density                  1    1963.1 4862294 86243
+ entropy_FusionHeat           1    1648.0 4862609 86244
+ wtd_gmean_FusionHeat         1    1568.7 4862688 86244
+ entropy_Density              1    1551.5 4862705 86244
+ wtd_range_atomic_radius      1    1479.7 4862777 86245
+ std_FusionHeat               1    1299.6 4862957 86245
+ wtd_range_atomic_mass        1    1227.7 4863029 86245
+ mean_FusionHeat              1     993.5 4863264 86246
+ wtd_entropy_atomic_radius    1     789.3 4863468 86247
+ wtd_mean_fie                 1     776.4 4863481 86247
<none>                                   4864257 86247
+ wtd_gmean_fie                1     568.0 4863689 86247
+ entropy_fie                  1     526.6 4863730 86248
+ mean_atomic_mass             1     473.7 4863783 86248
+ wtd_mean_Valence             1     379.5 4863877 86248
+ wtd_gmean_Valence            1     369.1 4863888 86248
+ gmean_FusionHeat             1     332.0 4863925 86248
+ mean_fie                     1     200.2 4864057 86249
+ wtd_gmean_atomic_mass        1     196.6 4864060 86249
+ gmean_atomic_radius          1     183.2 4864074 86249
+ entropy_ThermalConductivity  1     178.8 4864078 86249
+ gmean_fie                    1     168.3 4864089 86249
+ wtd_mean_atomic_mass         1     160.4 4864097 86249
+ gmean_atomic_mass            1     147.9 4864109 86249
+ gmean_Valence                1      88.9 4864168 86249
+ entropy_atomic_radius        1      77.1 4864180 86249
+ number_of_elements           1      26.7 4864230 86249
+ range_fie                    1       8.3 4864249 86249
+ mean_Valence                 1       6.2 4864251 86249
+ mean_atomic_radius           1       2.4 4864255 86249
+ wtd_gmean_Density            1       0.4 4864257 86249
```

```
Step:  AIC=86234.7
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density

                            Df Sum of Sq     RSS   AIC
+ mean_atomic_mass           1    9940.1 4849590 86206
+ wtd_gmean_Density          1    9515.1 4850015 86208
+ wtd_mean_atomic_radius     1    7610.3 4851920 86213
+ gmean_atomic_mass          1    7127.3 4852403 86215
+ wtd_gmean_atomic_radius    1    5280.5 4854250 86221
+ mean_ThermalConductivity   1    4468.6 4855062 86223
+ wtd_gmean_atomic_mass      1    4313.6 4855217 86223
+ wtd_mean_atomic_mass       1    4278.8 4855251 86224
+ range_FusionHeat           1    4130.6 4855400 86224
+ wtd_std_fie                1    3713.8 4855816 86225
+ wtd_std_Density            1    3366.9 4856163 86226
+ std_Density                1    2967.1 4856563 86228
+ entropy_Valence            1    2763.6 4856767 86228
+ wtd_mean_FusionHeat        1    2724.8 4856805 86228
+ std_Valence                1    2110.1 4857420 86230
+ std_fie                    1    2004.4 4857526 86231
+ gmean_Valence              1    1814.8 4857715 86231
+ entropy_Density            1    1592.3 4857938 86232
+ wtd_range_atomic_radius    1    1552.0 4857978 86232
+ entropy_FusionHeat         1    1520.8 4858009 86232
+ std_FusionHeat             1    1490.0 4858040 86232
+ mean_Valence               1    1290.4 4858240 86233
+ wtd_gmean_FusionHeat       1    1182.2 4858348 86233
+ mean_atomic_radius         1    1012.8 4858517 86234
+ gmean_Density              1    1004.9 4858525 86234
+ wtd_mean_Density           1     898.9 4858631 86234
+ wtd_range_atomic_mass      1     885.4 4858645 86234
<none>                                  4859530 86235
```

```
+ mean_FusionHeat              1     637.3 4858893 86235
+ wtd_entropy_atomic_radius    1     487.0 4859043 86235
+ wtd_mean_fie                 1     358.0 4859172 86236
+ wtd_gmean_fie                1     236.8 4859293 86236
+ gmean_atomic_radius          1     179.3 4859351 86236
+ entropy_fie                  1     148.9 4859381 86236
+ gmean_FusionHeat             1     140.4 4859390 86236
+ entropy_ThermalConductivity  1      80.9 4859449 86236
+ wtd_mean_Valence             1      30.5 4859500 86237
+ wtd_gmean_Valence            1      27.1 4859503 86237
+ gmean_fie                    1      26.9 4859503 86237
+ mean_fie                     1      26.6 4859504 86237
+ entropy_atomic_radius        1      26.0 4859504 86237
+ number_of_elements           1       6.2 4859524 86237
+ range_fie                    1       6.1 4859524 86237

Step:  AIC=86206.22
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass

                             Df Sum of Sq     RSS   AIC
+ wtd_gmean_Density            1    8902.4 4840688 86181
+ wtd_range_atomic_mass        1    8739.5 4840851 86181
+ entropy_Valence              1    5756.6 4843834 86191
+ gmean_Valence                1    5310.1 4844280 86192
+ std_Density                  1    5258.5 4844332 86192
+ wtd_mean_atomic_radius       1    5254.7 4844335 86192
+ wtd_std_fie                  1    4806.0 4844784 86193
+ mean_Valence                 1    4579.8 4845010 86194
+ range_FusionHeat             1    3560.6 4846029 86197
+ wtd_gmean_atomic_radius      1    3394.5 4846196 86198
+ std_fie                      1    2959.3 4846631 86199
+ entropy_Density              1    2749.8 4846840 86200
```

```
+ mean_ThermalConductivity     1    2567.5 4847023 86200
+ wtd_range_atomic_radius      1    2246.9 4847343 86201
+ gmean_atomic_mass            1    2236.5 4847354 86201
+ wtd_std_Density              1    2172.4 4847418 86202
+ entropy_FusionHeat           1    2126.4 4847464 86202
+ std_Valence                  1    2045.4 4847545 86202
+ entropy_fie                  1    1603.8 4847986 86203
+ std_FusionHeat               1    1462.5 4848128 86204
+ wtd_mean_Valence             1    1174.9 4848415 86205
+ wtd_mean_atomic_mass         1    1151.1 4848439 86205
+ wtd_gmean_Valence            1    1060.1 4848530 86205
+ gmean_fie                    1     884.5 4848706 86206
+ gmean_Density                1     807.3 4848783 86206
+ mean_fie                     1     734.6 4848856 86206
+ wtd_mean_Density             1     700.1 4848890 86206
<none>                                    4849590 86206
+ wtd_entropy_atomic_radius    1     595.0 4848995 86206
+ wtd_mean_FusionHeat          1     558.8 4849031 86207
+ wtd_gmean_atomic_mass        1     533.6 4849057 86207
+ gmean_FusionHeat             1     358.2 4849232 86207
+ wtd_gmean_fie                1     271.3 4849319 86207
+ entropy_atomic_radius        1     262.7 4849327 86207
+ mean_atomic_radius           1     137.6 4849453 86208
+ wtd_mean_fie                 1     115.5 4849475 86208
+ number_of_elements           1      94.4 4849496 86208
+ wtd_gmean_FusionHeat         1      56.2 4849534 86208
+ mean_FusionHeat              1      50.5 4849540 86208
+ gmean_atomic_radius          1      40.1 4849550 86208
+ range_fie                    1      13.2 4849577 86208
+ entropy_ThermalConductivity  1       7.6 4849583 86208

Step:  AIC=86180.87
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
```

```
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density

                              Df Sum of Sq     RSS   AIC
+ wtd_mean_atomic_mass         1    9767.9 4830920 86153
+ wtd_gmean_atomic_mass        1    8823.8 4831864 86156
+ wtd_range_atomic_mass        1    7807.1 4832881 86159
+ entropy_Valence              1    6924.5 4833763 86162
+ gmean_atomic_mass            1    6530.8 4834157 86163
+ std_Density                  1    6492.2 4834196 86163
+ wtd_mean_Density             1    5269.9 4835418 86167
+ gmean_Valence                1    3389.0 4837299 86172
+ wtd_mean_atomic_radius       1    3306.1 4837382 86173
+ entropy_Density              1    3262.9 4837425 86173
+ range_FusionHeat             1    3241.5 4837446 86173
+ mean_ThermalConductivity     1    3129.8 4837558 86173
+ wtd_std_fie                  1    2854.5 4837833 86174
+ mean_Valence                 1    2784.9 4837903 86174
+ entropy_fie                  1    2118.6 4838569 86176
+ entropy_FusionHeat           1    2072.6 4838615 86177
+ gmean_fie                    1    1925.6 4838762 86177
+ std_fie                      1    1820.6 4838867 86177
+ mean_fie                     1    1808.3 4838879 86177
+ std_Valence                  1    1760.4 4838927 86177
+ wtd_gmean_atomic_radius      1    1585.8 4839102 86178
+ gmean_Density                1    1314.8 4839373 86179
+ wtd_std_Density              1    1244.2 4839444 86179
+ std_FusionHeat               1    1231.1 4839457 86179
+ wtd_mean_FusionHeat          1     867.3 4839820 86180
+ wtd_range_atomic_radius      1     683.9 4840004 86181
<none>                                    4840688 86181
+ gmean_atomic_radius          1     469.6 4840218 86181
+ entropy_atomic_radius        1     302.4 4840385 86182
+ wtd_gmean_fie                1     300.7 4840387 86182
+ wtd_gmean_FusionHeat         1     271.6 4840416 86182
+ gmean_FusionHeat             1     262.9 4840425 86182
+ number_of_elements           1     223.6 4840464 86182
+ wtd_mean_fie                 1     202.4 4840485 86182
+ range_fie                    1     114.6 4840573 86183
+ mean_FusionHeat              1      81.9 4840606 86183
+ wtd_entropy_atomic_radius    1      18.6 4840669 86183
+ entropy_ThermalConductivity  1      17.6 4840670 86183
+ wtd_mean_Valence             1       2.7 4840685 86183
+ wtd_gmean_Valence            1       0.1 4840688 86183
+ mean_atomic_radius           1       0.0 4840688 86183

Step:  AIC=86152.81
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
```

```
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass

                            Df Sum of Sq     RSS   AIC
+ std_Density                1    8683.5 4822236 86128
+ entropy_Valence            1    6233.8 4824686 86136
+ gmean_Density              1    5186.9 4825733 86139
+ gmean_atomic_mass          1    4188.5 4826731 86142
+ mean_fie                   1    3928.6 4826991 86143
+ wtd_mean_atomic_radius     1    3693.1 4827227 86143
+ gmean_fie                  1    3580.1 4827340 86144
+ range_FusionHeat           1    3171.9 4827748 86145
+ gmean_Valence              1    2596.7 4828323 86147
+ wtd_mean_FusionHeat        1    2437.8 4828482 86147
+ mean_Valence               1    2090.5 4828829 86148
+ wtd_range_atomic_mass      1    1883.3 4829037 86149
+ std_Valence                1    1859.3 4829061 86149
+ wtd_gmean_FusionHeat       1    1841.8 4829078 86149
+ wtd_gmean_atomic_radius    1    1660.2 4829260 86150
+ range_fie                  1    1637.3 4829283 86150
+ entropy_fie                1    1550.6 4829369 86150
+ mean_ThermalConductivity   1    1334.8 4829585 86151
+ gmean_atomic_radius        1    1285.1 4829635 86151
+ wtd_mean_Density           1    1240.3 4829680 86151
+ wtd_std_Density            1    1213.3 4829707 86151
+ entropy_Density            1    1091.0 4829829 86151
+ std_FusionHeat             1    1023.0 4829897 86152
+ wtd_std_fie                1     822.6 4830097 86152
+ wtd_range_atomic_radius    1     805.9 4830114 86152
+ wtd_mean_fie               1     655.2 4830265 86153
<none>                                  4830920 86153
+ wtd_gmean_fie              1     640.7 4830279 86153
+ entropy_FusionHeat         1     579.4 4830340 86153
+ std_fie                    1     289.1 4830631 86154
```

```
+ number_of_elements           1     233.7 4830686 86154
+ mean_atomic_radius           1     135.4 4830785 86154
+ wtd_entropy_atomic_radius    1     121.4 4830799 86154
+ mean_FusionHeat              1     101.1 4830819 86154
+ gmean_FusionHeat             1      86.4 4830834 86155
+ entropy_atomic_radius        1      31.3 4830889 86155
+ wtd_gmean_atomic_mass        1      16.2 4830904 86155
+ entropy_ThermalConductivity  1      14.8 4830905 86155
+ wtd_mean_Valence             1       1.3 4830919 86155
+ wtd_gmean_Valence            1       0.4 4830920 86155

Step:  AIC=86128.03
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density

                             Df Sum of Sq     RSS   AIC
+ wtd_std_Density             1    7771.4 4814465 86106
+ gmean_atomic_mass           1    7254.4 4814982 86108
+ entropy_Valence             1    6402.5 4815834 86110
+ gmean_Density               1    4526.0 4817710 86116
+ mean_fie                    1    3998.7 4818238 86118
+ gmean_fie                   1    3621.6 4818615 86119
+ wtd_mean_atomic_radius      1    3260.9 4818975 86120
+ entropy_Density             1    2963.5 4819273 86121
+ gmean_Valence               1    2459.4 4819777 86122
+ wtd_mean_FusionHeat         1    2357.8 4819879 86123
+ mean_ThermalConductivity    1    2324.4 4819912 86123
+ mean_Valence                1    2009.7 4820227 86124
+ range_FusionHeat            1    1998.1 4820238 86124
+ gmean_atomic_radius         1    1817.5 4820419 86124
+ std_Valence                 1    1796.9 4820440 86124
+ wtd_gmean_FusionHeat        1    1697.5 4820539 86125
```

```
+ wtd_range_atomic_mass        1    1514.4 4820722 86125
+ entropy_fie                  1    1508.8 4820728 86125
+ wtd_gmean_atomic_radius      1    1294.5 4820942 86126
+ range_fie                    1    1285.0 4820951 86126
+ wtd_mean_Density             1    1173.3 4821063 86126
+ wtd_range_atomic_radius      1     962.7 4821274 86127
+ wtd_std_fie                  1     913.1 4821323 86127
+ wtd_gmean_atomic_mass        1     862.6 4821374 86127
+ wtd_mean_fie                 1     750.5 4821486 86128
+ wtd_gmean_fie                1     710.6 4821526 86128
<none>                                   4822236 86128
+ entropy_FusionHeat           1     614.4 4821622 86128
+ std_FusionHeat               1     497.7 4821739 86128
+ std_fie                      1     414.8 4821822 86129
+ mean_atomic_radius           1     268.6 4821968 86129
+ number_of_elements           1     168.0 4822068 86130
+ wtd_entropy_atomic_radius    1      93.0 4822143 86130
+ gmean_FusionHeat             1      52.6 4822184 86130
+ wtd_gmean_Valence            1      42.7 4822194 86130
+ entropy_ThermalConductivity  1      25.7 4822211 86130
+ entropy_atomic_radius        1      23.5 4822213 86130
+ mean_FusionHeat              1      20.1 4822216 86130
+ wtd_mean_Valence             1      12.6 4822224 86130

Step:  AIC=86106.03
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density

                            Df Sum of Sq     RSS   AIC
+ entropy_Density            1    8476.8 4805988 86082
+ entropy_Valence            1    7942.5 4806522 86083
+ gmean_atomic_mass          1    7880.6 4806584 86084
```

```
+ mean_fie                     1    3464.5 4811000 86097
+ gmean_fie                    1    3433.0 4811032 86097
+ wtd_mean_atomic_radius       1    3049.2 4811416 86099
+ gmean_Valence                1    2925.0 4811540 86099
+ mean_ThermalConductivity     1    2762.1 4811703 86099
+ wtd_range_atomic_mass        1    2646.2 4811819 86100
+ wtd_std_fie                  1    2456.8 4812008 86100
+ mean_Valence                 1    2449.1 4812016 86100
+ entropy_fie                  1    2434.4 4812031 86100
+ gmean_Density                1    2401.6 4812063 86101
+ wtd_mean_FusionHeat          1    1735.9 4812729 86103
+ range_FusionHeat             1    1556.6 4812908 86103
+ gmean_atomic_radius          1    1500.3 4812965 86103
+ wtd_range_atomic_radius      1    1402.6 4813062 86104
+ wtd_gmean_atomic_mass        1    1396.1 4813069 86104
+ wtd_gmean_atomic_radius      1    1282.2 4813183 86104
+ std_fie                      1    1245.0 4813220 86104
+ std_Valence                  1    1184.6 4813280 86104
+ wtd_gmean_FusionHeat         1    1110.7 4813354 86105
+ entropy_FusionHeat           1     920.1 4813545 86105
+ wtd_gmean_fie                1     857.6 4813607 86105
+ wtd_mean_fie                 1     692.6 4813772 86106
<none>                                   4814465 86106
+ range_fie                    1     388.1 4814077 86107
+ std_FusionHeat               1     322.9 4814142 86107
+ entropy_atomic_radius        1     285.8 4814179 86107
+ number_of_elements           1     276.2 4814189 86107
+ mean_atomic_radius           1     222.4 4814243 86107
+ wtd_mean_Valence             1     162.9 4814302 86108
+ wtd_entropy_atomic_radius    1     117.8 4814347 86108
+ wtd_gmean_Valence            1      89.2 4814376 86108
+ gmean_FusionHeat             1      56.4 4814409 86108
+ wtd_mean_Density             1      29.9 4814435 86108
+ mean_FusionHeat              1      15.6 4814449 86108
+ entropy_ThermalConductivity  1       7.3 4814458 86108

Step:  AIC=86081.8
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
```

```
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density

                             Df Sum of Sq     RSS   AIC
+ gmean_atomic_mass            1    7195.0 4798793 86061
+ mean_fie                     1    5728.6 4800260 86066
+ entropy_Valence              1    5264.7 4800723 86067
+ gmean_fie                    1    4694.9 4801293 86069
+ wtd_mean_atomic_radius       1    3360.3 4802628 86073
+ gmean_Valence                1    2481.4 4803507 86076
+ gmean_Density                1    2388.6 4803600 86076
+ wtd_mean_FusionHeat          1    2345.3 4803643 86077
+ range_FusionHeat             1    2229.3 4803759 86077
+ mean_Valence                 1    2082.0 4803906 86077
+ range_fie                    1    2047.4 4803941 86077
+ wtd_range_atomic_mass        1    1828.4 4804160 86078
+ wtd_gmean_FusionHeat         1    1796.4 4804192 86078
+ std_Valence                  1    1670.5 4804318 86079
+ gmean_atomic_radius          1    1580.2 4804408 86079
+ mean_ThermalConductivity     1    1520.9 4804467 86079
+ wtd_mean_fie                 1    1375.6 4804613 86080
+ wtd_gmean_atomic_radius      1    1367.0 4804621 86080
+ wtd_gmean_fie                1    1294.9 4804693 86080
+ wtd_range_atomic_radius      1    1248.3 4804740 86080
+ wtd_gmean_atomic_mass        1    1217.1 4804771 86080
+ entropy_fie                  1     984.7 4805004 86081
+ wtd_std_fie                  1     767.6 4805221 86081
<none>                                    4805988 86082
+ std_FusionHeat               1     636.6 4805352 86082
+ wtd_mean_Valence             1     385.8 4805602 86083
+ wtd_entropy_atomic_radius    1     317.1 4805671 86083
+ gmean_FusionHeat             1     255.6 4805733 86083
+ wtd_gmean_Valence            1     248.3 4805740 86083
+ mean_FusionHeat              1     197.0 4805791 86083
+ mean_atomic_radius           1     194.9 4805793 86083
+ entropy_ThermalConductivity  1     150.5 4805838 86083
+ number_of_elements           1     115.9 4805872 86083
+ std_fie                      1      36.9 4805951 86084
+ entropy_FusionHeat           1      27.2 4805961 86084
+ entropy_atomic_radius        1      16.0 4805972 86084
+ wtd_mean_Density             1       0.9 4805987 86084

Step:  AIC=86061.5
```

```
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass

                            Df Sum of Sq     RSS   AIC
+ wtd_mean_atomic_radius     1    4430.0 4794363 86050
+ mean_fie                   1    4384.7 4794409 86050
+ gmean_fie                  1    3487.4 4795306 86053
+ wtd_mean_FusionHeat        1    3045.6 4795748 86054
+ wtd_gmean_atomic_mass      1    2883.1 4795910 86055
+ wtd_gmean_FusionHeat       1    2645.3 4796148 86055
+ gmean_Valence              1    2636.4 4796157 86055
+ range_FusionHeat           1    2491.9 4796301 86056
+ entropy_Valence            1    2301.2 4796492 86056
+ wtd_gmean_atomic_radius    1    2201.9 4796591 86057
+ mean_Valence               1    2157.9 4796635 86057
+ range_fie                  1    2139.2 4796654 86057
+ wtd_range_atomic_mass      1    1653.3 4797140 86058
+ std_Valence                1    1404.2 4797389 86059
+ mean_ThermalConductivity   1    1068.3 4797725 86060
+ entropy_atomic_radius      1    1039.0 4797754 86060
+ wtd_range_atomic_radius    1     911.3 4797882 86061
+ wtd_mean_fie               1     839.4 4797954 86061
+ wtd_gmean_fie              1     753.7 4798040 86061
+ gmean_Density              1     668.9 4798124 86061
+ std_FusionHeat             1     649.0 4798144 86061
<none>                                   4798793 86061
+ gmean_atomic_radius        1     583.4 4798210 86062
+ gmean_FusionHeat           1     565.7 4798228 86062
+ wtd_std_fie                1     478.4 4798315 86062
+ wtd_mean_Density           1     463.2 4798330 86062
+ mean_FusionHeat            1     353.0 4798440 86062
```

```
+ wtd_mean_Valence             1     327.0 4798466 86062
+ entropy_FusionHeat           1     227.0 4798566 86063
+ wtd_gmean_Valence            1     220.9 4798572 86063
+ wtd_entropy_atomic_radius    1     187.7 4798605 86063
+ number_of_elements           1     143.4 4798650 86063
+ entropy_ThermalConductivity  1      48.1 4798745 86063
+ std_fie                      1      30.4 4798763 86063
+ entropy_fie                  1      10.4 4798783 86063
+ mean_atomic_radius           1       0.0 4798793 86063

Step:  AIC=86049.75
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius

                            Df Sum of Sq     RSS   AIC
+ wtd_gmean_atomic_radius    1     31695 4762668 85953
+ gmean_atomic_radius        1     12399 4781964 86013
+ mean_fie                   1     11188 4783175 86017
+ gmean_fie                  1      9891 4784472 86021
+ wtd_range_atomic_radius    1      6869 4787494 86030
+ wtd_gmean_fie              1      6453 4787910 86032
+ wtd_mean_fie               1      6327 4788037 86032
+ mean_atomic_radius         1      5830 4788533 86034
+ entropy_Valence            1      4020 4790343 86039
+ gmean_Valence              1      2580 4791783 86044
+ wtd_mean_FusionHeat        1      2542 4791821 86044
+ wtd_gmean_atomic_mass      1      2517 4791846 86044
+ range_fie                  1      2318 4792046 86045
+ range_FusionHeat           1      2192 4792171 86045
+ wtd_gmean_FusionHeat       1      2160 4792204 86045
+ mean_Valence               1      2071 4792292 86045
```

```
+ std_Valence                  1      1548 4792815 86047
+ wtd_range_atomic_mass        1      1240 4793123 86048
+ wtd_entropy_atomic_radius    1      1236 4793127 86048
<none>                                    4794363 86050
+ wtd_mean_Density             1       544 4793819 86050
+ gmean_FusionHeat             1       526 4793838 86050
+ std_FusionHeat               1       489 4793874 86050
+ gmean_Density                1       458 4793905 86050
+ entropy_atomic_radius        1       442 4793921 86050
+ wtd_std_fie                  1       430 4793933 86050
+ wtd_mean_Valence             1       420 4793944 86050
+ entropy_fie                  1       340 4794024 86051
+ mean_ThermalConductivity     1       313 4794050 86051
+ wtd_gmean_Valence            1       307 4794056 86051
+ mean_FusionHeat              1       295 4794069 86051
+ entropy_FusionHeat           1       236 4794127 86051
+ number_of_elements           1        15 4794349 86052
+ entropy_ThermalConductivity  1        13 4794350 86052
+ std_fie                      1        13 4794351 86052

Step:  AIC=85953.03
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius

                             Df Sum of Sq     RSS   AIC
+ wtd_std_fie                 1   11533.4 4751135 85919
+ gmean_atomic_radius         1    9033.1 4753635 85927
+ wtd_range_atomic_radius     1    8751.3 4753917 85928
+ mean_atomic_radius          1    8176.4 4754492 85929
+ wtd_mean_Density            1    7681.1 4754987 85931
+ std_fie                     1    7011.6 4755657 85933
```

```
+ gmean_fie                    1    7005.4 4755663 85933
+ mean_fie                     1    5826.3 4756842 85937
+ entropy_Valence              1    4817.2 4757851 85940
+ wtd_mean_FusionHeat          1    4630.4 4758038 85941
+ wtd_gmean_atomic_mass        1    4436.8 4758232 85941
+ gmean_Valence                1    4203.3 4758465 85942
+ range_FusionHeat             1    3969.3 4758699 85943
+ mean_Valence                 1    3535.2 4759133 85944
+ wtd_gmean_fie                1    3264.3 4759404 85945
+ wtd_gmean_FusionHeat         1    3015.0 4759654 85946
+ wtd_entropy_atomic_radius    1    2801.3 4759867 85946
+ entropy_fie                  1    1831.8 4760837 85949
+ wtd_mean_fie                 1    1668.1 4761000 85950
+ std_FusionHeat               1    1493.3 4761175 85950
+ range_fie                    1    1096.4 4761572 85952
+ std_Valence                  1     963.0 4761706 85952
+ mean_FusionHeat              1     919.1 4761749 85952
+ gmean_Density                1     831.9 4761837 85952
<none>                                   4762668 85953
+ gmean_FusionHeat             1     557.3 4762111 85953
+ wtd_mean_Valence             1     541.1 4762127 85953
+ wtd_gmean_Valence            1     460.1 4762208 85954
+ wtd_range_atomic_mass        1     423.6 4762245 85954
+ entropy_ThermalConductivity  1     243.8 4762425 85954
+ entropy_atomic_radius        1     216.0 4762452 85954
+ number_of_elements           1      96.8 4762572 85955
+ mean_ThermalConductivity     1      69.5 4762599 85955
+ entropy_FusionHeat           1       7.0 4762662 85955

Step:  AIC=85918.94
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
```

```
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie

                             Df Sum of Sq     RSS   AIC
+ wtd_range_atomic_radius     1   10208.8 4740926 85889
+ gmean_atomic_radius         1    9896.3 4741239 85890
+ mean_atomic_radius          1    9118.6 4742017 85892
+ mean_fie                    1    8857.4 4742278 85893
+ gmean_fie                   1    8005.2 4743130 85896
+ range_fie                   1    7916.0 4743219 85896
+ wtd_mean_FusionHeat         1    7243.9 4743891 85898
+ wtd_gmean_FusionHeat        1    5958.6 4745177 85902
+ entropy_Valence             1    5931.5 4745204 85902
+ wtd_mean_fie                1    5498.9 4745636 85904
+ wtd_gmean_fie               1    5449.2 4745686 85904
+ wtd_entropy_atomic_radius   1    4685.9 4746449 85906
+ wtd_gmean_atomic_mass       1    4183.8 4746951 85908
+ range_FusionHeat            1    3633.0 4747502 85910
+ wtd_mean_Density            1    3344.6 4747791 85910
+ gmean_Valence               1    3086.5 4748049 85911
+ mean_Valence                1    2535.7 4748599 85913
+ std_Valence                 1    2307.5 4748828 85914
+ gmean_FusionHeat            1    2170.1 4748965 85914
+ mean_FusionHeat             1    2118.6 4749016 85914
+ std_FusionHeat              1    1178.2 4749957 85917
+ entropy_fie                 1    1130.5 4750005 85917
+ wtd_range_atomic_mass       1    1025.4 4750110 85918
<none>                                   4751135 85919
+ wtd_mean_Valence            1     539.0 4750596 85919
+ entropy_atomic_radius       1     395.8 4750739 85920
+ wtd_gmean_Valence           1     357.3 4750778 85920
+ entropy_ThermalConductivity 1     218.6 4750917 85920
+ std_fie                     1     158.4 4750977 85920
+ entropy_FusionHeat          1      79.6 4751056 85921
+ number_of_elements          1      26.8 4751108 85921
+ mean_ThermalConductivity    1      17.5 4751118 85921
+ gmean_Density               1       9.0 4751126 85921

Step:  AIC=85888.93
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
```

```
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius

                              Df Sum of Sq     RSS   AIC
+ gmean_atomic_radius          1   21967.6 4718959 85822
+ mean_atomic_radius           1   21504.2 4719422 85823
+ mean_fie                     1   12903.8 4728023 85850
+ gmean_fie                    1   11949.7 4728977 85853
+ entropy_Valence              1    8600.2 4732326 85864
+ range_fie                    1    7319.1 4733607 85868
+ wtd_mean_FusionHeat          1    7185.5 4733741 85868
+ wtd_gmean_FusionHeat         1    5916.6 4735010 85872
+ wtd_gmean_fie                1    5257.3 4735669 85874
+ wtd_mean_fie                 1    5248.0 4735678 85874
+ wtd_gmean_atomic_mass        1    4554.3 4736372 85877
+ wtd_mean_Density             1    4074.1 4736852 85878
+ range_FusionHeat             1    3275.6 4737651 85881
+ gmean_Valence                1    2678.5 4738248 85883
+ entropy_fie                  1    2296.7 4738630 85884
+ gmean_FusionHeat             1    2115.2 4738811 85884
+ mean_Valence                 1    2045.0 4738881 85885
+ mean_FusionHeat              1    1898.3 4739028 85885
+ std_Valence                  1    1607.3 4739319 85886
+ entropy_atomic_radius        1     802.9 4740123 85888
+ std_FusionHeat               1     771.6 4740155 85889
<none>                                     4740926 85889
+ entropy_ThermalConductivity  1     473.0 4740453 85889
+ wtd_entropy_atomic_radius    1     375.7 4740551 85890
+ std_fie                      1     218.6 4740708 85890
+ entropy_FusionHeat           1     112.2 4740814 85891
+ wtd_range_atomic_mass        1     111.2 4740815 85891
+ wtd_mean_Valence             1     101.8 4740825 85891
+ gmean_Density                1      66.3 4740860 85891
+ wtd_gmean_Valence            1      60.9 4740865 85891
+ number_of_elements           1      18.8 4740908 85891
+ mean_ThermalConductivity     1       8.6 4740918 85891

Step:  AIC=85821.8
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
```

```
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius

                              Df Sum of Sq     RSS   AIC
+ wtd_entropy_atomic_radius    1   14935.0 4704024 85777
+ entropy_Valence              1    8958.5 4710000 85796
+ range_FusionHeat             1    7860.8 4711098 85799
+ wtd_mean_FusionHeat          1    7134.7 4711824 85801
+ wtd_mean_Density             1    5927.1 4713032 85805
+ wtd_gmean_FusionHeat         1    5795.1 4713164 85806
+ entropy_atomic_radius        1    4582.0 4714377 85809
+ wtd_mean_fie                 1    4516.1 4714443 85810
+ wtd_gmean_fie                1    4447.7 4714511 85810
+ std_FusionHeat               1    4145.3 4714813 85811
+ entropy_fie                  1    4101.7 4714857 85811
+ gmean_Density                1    3709.7 4715249 85812
+ mean_fie                     1    3218.4 4715740 85814
+ range_fie                    1    3061.5 4715897 85814
+ std_Valence                  1    2960.9 4715998 85814
+ gmean_fie                    1    2945.6 4716013 85815
+ mean_FusionHeat              1    2802.4 4716156 85815
+ wtd_range_atomic_mass        1    2620.2 4716338 85816
+ gmean_FusionHeat             1    1995.8 4716963 85818
+ entropy_ThermalConductivity  1    1715.0 4717244 85818
+ wtd_gmean_atomic_mass        1    1589.2 4717370 85819
+ gmean_Valence                1    1242.8 4717716 85820
+ mean_Valence                 1     955.4 4718003 85821
<none>                                    4718959 85822
+ entropy_FusionHeat           1     472.4 4718486 85822
+ std_fie                      1     295.3 4718663 85823
+ mean_ThermalConductivity     1     228.8 4718730 85823
```

```
+ wtd_gmean_Valence            1      96.0 4718863 85823
+ wtd_mean_Valence             1      27.5 4718931 85824
+ number_of_elements           1      26.7 4718932 85824
+ mean_atomic_radius           1       5.9 4718953 85824

Step:  AIC=85776.62
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius

                              Df Sum of Sq     RSS   AIC
+ wtd_mean_FusionHeat          1    5799.1 4698225 85760
+ wtd_gmean_atomic_mass        1    5521.7 4698502 85761
+ entropy_Valence              1    5370.5 4698653 85762
+ wtd_mean_Density             1    4611.4 4699412 85764
+ range_FusionHeat             1    4258.1 4699766 85765
+ wtd_gmean_FusionHeat         1    3977.3 4700046 85766
+ wtd_gmean_fie                1    3754.4 4700269 85767
+ wtd_mean_fie                 1    3714.2 4700310 85767
+ gmean_Valence                1    3645.2 4700378 85767
+ mean_fie                     1    3043.7 4700980 85769
+ mean_Valence                 1    3022.5 4701001 85769
+ gmean_fie                    1    2898.1 4701126 85769
+ range_fie                    1    2625.4 4701398 85770
+ gmean_Density                1    2164.3 4701859 85772
+ entropy_ThermalConductivity  1    1893.5 4702130 85773
+ mean_FusionHeat              1    1605.4 4702418 85774
+ gmean_FusionHeat             1    1522.6 4702501 85774
+ std_Valence                  1    1478.5 4702545 85774
+ std_FusionHeat               1    1345.3 4702678 85774
```

```
+ entropy_atomic_radius        1     964.9 4703059 85776
+ entropy_fie                  1     879.8 4703144 85776
+ wtd_range_atomic_mass        1     800.0 4703224 85776
<none>                                     4704024 85777
+ std_fie                      1     308.9 4703715 85778
+ wtd_mean_Valence             1      96.9 4703927 85778
+ mean_ThermalConductivity     1      74.6 4703949 85778
+ wtd_gmean_Valence            1      70.7 4703953 85778
+ number_of_elements           1      51.6 4703972 85778
+ entropy_FusionHeat           1      30.6 4703993 85779
+ mean_atomic_radius           1      23.1 4704001 85779

Step:  AIC=85760.26
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat

                             Df Sum of Sq     RSS   AIC
+ wtd_gmean_fie               1    5932.4 4692292 85743
+ wtd_mean_fie                1    5890.1 4692334 85744
+ entropy_Valence             1    5604.4 4692620 85744
+ wtd_gmean_atomic_mass       1    5463.9 4692761 85745
+ gmean_Valence               1    4740.0 4693485 85747
+ mean_fie                    1    4645.5 4693579 85748
+ wtd_mean_Density            1    4632.9 4693592 85748
+ gmean_fie                   1    4314.0 4693911 85749
+ range_FusionHeat            1    4267.9 4693957 85749
+ mean_Valence                1    3906.2 4694318 85750
+ range_fie                   1    3337.1 4694888 85752
+ gmean_Density               1    2409.8 4695815 85755
```

```
+ mean_FusionHeat              1    2101.0 4696124 85756
+ gmean_FusionHeat             1    2099.1 4696125 85756
+ entropy_ThermalConductivity  1    1902.6 4696322 85756
+ std_Valence                  1    1851.7 4696373 85756
+ std_FusionHeat               1    1574.3 4696650 85757
+ wtd_range_atomic_mass        1    1475.6 4696749 85758
+ wtd_gmean_FusionHeat         1    1353.1 4696871 85758
+ entropy_atomic_radius        1     816.5 4697408 85760
+ entropy_fie                  1     689.5 4697535 85760
<none>                                    4698225 85760
+ entropy_FusionHeat           1     399.5 4697825 85761
+ wtd_mean_Valence             1     395.1 4697829 85761
+ wtd_gmean_Valence            1     364.3 4697860 85761
+ std_fie                      1     159.4 4698065 85762
+ mean_atomic_radius           1     149.6 4698075 85762
+ number_of_elements           1      49.1 4698175 85762
+ mean_ThermalConductivity     1       3.7 4698221 85762

Step:  AIC=85743.45
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie

                            Df Sum of Sq     RSS   AIC
+ wtd_mean_Density           1    6519.5 4685773 85725
+ entropy_Valence            1    5751.6 4686541 85727
+ wtd_gmean_atomic_mass      1    5445.1 4686847 85728
+ range_FusionHeat           1    4276.0 4688016 85732
+ gmean_Valence              1    3753.5 4688539 85734
+ gmean_Density              1    3657.4 4688635 85734
```

```
+ range_fie                    1    3489.4 4688803 85734
+ mean_Valence                 1    2972.4 4689320 85736
+ gmean_FusionHeat             1    2585.8 4689706 85737
+ wtd_gmean_FusionHeat         1    2569.5 4689723 85737
+ entropy_ThermalConductivity  1    2532.5 4689760 85737
+ mean_FusionHeat              1    1923.7 4690368 85739
+ wtd_range_atomic_mass        1    1836.6 4690456 85740
+ std_Valence                  1    1639.8 4690652 85740
+ std_FusionHeat               1    1615.4 4690677 85740
+ entropy_atomic_radius        1     921.7 4691370 85743
<none>                                   4692292 85743
+ entropy_fie                  1     508.3 4691784 85744
+ entropy_FusionHeat           1     403.6 4691889 85744
+ number_of_elements           1     348.5 4691944 85744
+ mean_atomic_radius           1     183.7 4692108 85745
+ mean_fie                     1     175.1 4692117 85745
+ wtd_mean_Valence             1     107.7 4692184 85745
+ wtd_gmean_Valence            1      98.3 4692194 85745
+ gmean_fie                    1      86.0 4692206 85745
+ std_fie                      1      51.3 4692241 85745
+ mean_ThermalConductivity     1       0.2 4692292 85745
+ wtd_mean_fie                 1       0.0 4692292 85745

Step:  AIC=85724.76
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density

                              Df Sum of Sq     RSS   AIC
```

```
+ entropy_Valence              1    5392.4 4680380 85710
+ gmean_Valence                1    4188.8 4681584 85713
+ range_FusionHeat             1    4056.8 4681716 85714
+ wtd_gmean_atomic_mass        1    3749.0 4682024 85715
+ mean_Valence                 1    3354.2 4682418 85716
+ range_fie                    1    3221.5 4682551 85717
+ std_Valence                  1    2049.9 4683723 85720
+ entropy_ThermalConductivity  1    1896.2 4683876 85721
+ std_FusionHeat               1    1452.1 4684321 85722
+ mean_FusionHeat              1    1307.9 4684465 85723
+ gmean_FusionHeat             1    1291.2 4684481 85723
+ wtd_gmean_FusionHeat         1    1212.6 4684560 85723
+ entropy_atomic_radius        1     895.5 4684877 85724
<none>                                    4685773 85725
+ wtd_mean_Valence             1     460.9 4685312 85725
+ wtd_gmean_Valence            1     448.0 4685325 85725
+ entropy_fie                  1     375.5 4685397 85726
+ gmean_Density                1     350.5 4685422 85726
+ wtd_range_atomic_mass        1     323.1 4685449 85726
+ entropy_FusionHeat           1     231.7 4685541 85726
+ number_of_elements           1     190.1 4685582 85726
+ mean_atomic_radius           1     189.7 4685583 85726
+ std_fie                      1     146.6 4685626 85726
+ wtd_mean_fie                 1      47.2 4685725 85727
+ mean_ThermalConductivity     1      10.3 4685762 85727
+ gmean_fie                    1       5.4 4685767 85727
+ mean_fie                     1       0.5 4685772 85727

Step:  AIC=85709.62
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
```

```
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence

                              Df Sum of Sq     RSS   AIC
+ entropy_fie                  1    6655.9 4673724 85690
+ range_FusionHeat             1    4197.6 4676183 85698
+ range_fie                    1    3655.0 4676725 85700
+ gmean_Valence                1    3332.5 4677048 85701
+ wtd_gmean_atomic_mass        1    3310.4 4677070 85701
+ mean_Valence                 1    2915.5 4677465 85702
+ entropy_atomic_radius        1    2632.4 4677748 85703
+ number_of_elements           1    2263.6 4678117 85704
+ mean_FusionHeat              1    1462.9 4678917 85707
+ wtd_gmean_FusionHeat         1    1341.2 4679039 85707
+ std_FusionHeat               1    1222.7 4679157 85708
+ gmean_FusionHeat             1    1160.0 4679220 85708
+ std_Valence                  1    1086.8 4679293 85708
+ entropy_ThermalConductivity  1     755.2 4679625 85709
<none>                                    4680380 85710
+ mean_atomic_radius           1     566.0 4679814 85710
+ wtd_range_atomic_mass        1     411.4 4679969 85710
+ wtd_mean_Valence             1     302.3 4680078 85711
+ gmean_fie                    1     255.0 4680125 85711
+ wtd_gmean_Valence            1     249.9 4680130 85711
+ mean_fie                     1     192.1 4680188 85711
+ wtd_mean_fie                 1     152.3 4680228 85711
+ mean_ThermalConductivity     1      67.7 4680312 85711
+ std_fie                      1      57.3 4680323 85711
+ entropy_FusionHeat           1      23.2 4680357 85712
+ gmean_Density                1       0.3 4680380 85712

Step:  AIC=85690.44
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
```

```
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie

                              Df Sum of Sq     RSS   AIC
+ range_fie                    1    3401.2 4670323 85682
+ range_FusionHeat             1    3301.2 4670423 85682
+ wtd_gmean_atomic_mass        1    2836.3 4670888 85683
+ entropy_ThermalConductivity  1    2003.2 4671721 85686
+ mean_Valence                 1    1571.0 4672153 85687
+ gmean_Valence                1    1386.5 4672338 85688
+ wtd_gmean_FusionHeat         1    1152.3 4672572 85689
+ mean_FusionHeat              1    1144.7 4672580 85689
+ std_FusionHeat               1     713.0 4673011 85690
+ gmean_FusionHeat             1     655.8 4673068 85690
+ entropy_atomic_radius        1     640.1 4673084 85690
<none>                                   4673724 85690
+ number_of_elements           1     425.7 4673299 85691
+ std_fie                      1     364.5 4673360 85691
+ wtd_range_atomic_mass        1     357.4 4673367 85691
+ std_Valence                  1     353.9 4673370 85691
+ wtd_mean_fie                 1     345.7 4673379 85691
+ entropy_FusionHeat           1     178.8 4673545 85692
+ mean_atomic_radius           1      16.7 4673708 85692
+ wtd_mean_Valence             1      12.6 4673712 85692
+ gmean_fie                    1       6.8 4673717 85692
+ mean_fie                     1       6.4 4673718 85692
+ mean_ThermalConductivity     1       5.6 4673719 85692
+ wtd_gmean_Valence            1       3.4 4673721 85692
+ gmean_Density                1       1.7 4673723 85692

Step:  AIC=85681.6
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
```

```
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie

                              Df Sum of Sq     RSS   AIC
+ std_fie                      1   14899.4 4655424 85636
+ range_FusionHeat             1    3916.1 4666407 85671
+ wtd_gmean_atomic_mass        1    2661.1 4667662 85675
+ mean_Valence                 1    2183.9 4668139 85677
+ gmean_Valence                1    2076.2 4668247 85677
+ entropy_ThermalConductivity  1    1977.3 4668346 85677
+ mean_FusionHeat              1    1517.7 4668805 85679
+ number_of_elements           1    1175.5 4669148 85680
+ wtd_gmean_FusionHeat         1    1137.5 4669186 85680
+ gmean_FusionHeat             1    1131.2 4669192 85680
+ std_FusionHeat               1     984.4 4669339 85680
<none>                                    4670323 85682
+ wtd_range_atomic_mass        1     397.6 4669925 85682
+ entropy_atomic_radius        1     341.2 4669982 85683
+ std_Valence                  1     296.4 4670027 85683
+ mean_atomic_radius           1     246.1 4670077 85683
+ mean_fie                     1     113.1 4670210 85683
+ wtd_mean_Valence             1     101.0 4670222 85683
+ wtd_mean_fie                 1      54.8 4670268 85683
+ gmean_Density                1      47.0 4670276 85683
+ entropy_FusionHeat           1      34.8 4670288 85683
+ wtd_gmean_Valence            1      22.2 4670301 85684
+ gmean_fie                    1       7.1 4670316 85684
+ mean_ThermalConductivity     1       0.0 4670323 85684

Step:  AIC=85636.04
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
```

```
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie

                              Df Sum of Sq     RSS   AIC
+ number_of_elements           1    3537.2 4651886 85627
+ range_FusionHeat             1    2948.0 4652476 85629
+ wtd_gmean_atomic_mass        1    2783.4 4652640 85629
+ entropy_ThermalConductivity  1    1929.2 4653494 85632
+ entropy_atomic_radius        1    1901.1 4653523 85632
+ mean_Valence                 1    1729.1 4653695 85633
+ gmean_Valence                1    1544.6 4653879 85633
+ mean_FusionHeat              1    1291.8 4654132 85634
+ wtd_gmean_FusionHeat         1    1217.5 4654206 85634
<none>                                    4655424 85636
+ gmean_FusionHeat             1     619.4 4654804 85636
+ wtd_mean_fie                 1     590.8 4654833 85636
+ wtd_range_atomic_mass        1     470.2 4654953 85637
+ entropy_FusionHeat           1     352.5 4655071 85637
+ std_FusionHeat               1     344.8 4655079 85637
+ gmean_fie                    1     327.8 4655096 85637
+ mean_fie                     1     279.8 4655144 85637
+ mean_atomic_radius           1      70.3 4655353 85638
+ wtd_mean_Valence             1      51.5 4655372 85638
+ gmean_Density                1      23.5 4655400 85638
+ wtd_gmean_Valence            1       4.5 4655419 85638
+ mean_ThermalConductivity     1       0.7 4655423 85638
+ std_Valence                  1       0.1 4655424 85638

Step:  AIC=85626.73
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
```

```
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements

                              Df Sum of Sq     RSS   AIC
+ wtd_gmean_atomic_mass        1   3137.51 4648749 85619
+ range_FusionHeat             1   2492.24 4649394 85621
+ entropy_atomic_radius        1   1863.98 4650022 85623
+ entropy_ThermalConductivity  1   1735.97 4650150 85623
+ mean_Valence                 1   1691.35 4650195 85623
+ gmean_Valence                1   1515.85 4650371 85624
+ mean_FusionHeat              1   1321.07 4650565 85625
+ wtd_gmean_FusionHeat         1   1127.60 4650759 85625
<none>                                   4651886 85627
+ gmean_FusionHeat             1    548.90 4651338 85627
+ wtd_range_atomic_mass        1    525.86 4651361 85627
+ wtd_mean_fie                 1    459.91 4651427 85627
+ entropy_FusionHeat           1    434.99 4651451 85627
+ gmean_fie                    1    395.46 4651491 85627
+ mean_fie                     1    296.21 4651590 85628
+ std_FusionHeat               1    248.48 4651638 85628
+ gmean_Density                1    161.99 4651724 85628
+ mean_atomic_radius           1    107.46 4651779 85628
+ wtd_mean_Valence             1     29.13 4651857 85629
+ std_Valence                  1     28.67 4651858 85629
+ mean_ThermalConductivity     1      1.41 4651885 85629
+ wtd_gmean_Valence            1      0.05 4651886 85629

Step:  AIC=85618.69
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
```

```
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass

                             Df Sum of Sq     RSS   AIC
+ range_FusionHeat             1   2284.34 4646465 85613
+ entropy_ThermalConductivity  1   2015.37 4646734 85614
+ entropy_atomic_radius        1   1978.50 4646770 85614
+ wtd_gmean_FusionHeat         1   1570.68 4647178 85616
+ mean_Valence                 1   1528.98 4647220 85616
+ gmean_Valence                1   1367.81 4647381 85616
+ mean_FusionHeat              1   1233.36 4647516 85617
<none>                                   4648749 85619
+ gmean_Density                1    533.70 4648215 85619
+ gmean_FusionHeat             1    522.51 4648226 85619
+ entropy_FusionHeat           1    433.09 4648316 85619
+ wtd_range_atomic_mass        1    414.02 4648335 85619
+ gmean_fie                    1    351.61 4648397 85620
+ wtd_mean_fie                 1    342.74 4648406 85620
+ mean_fie                     1    255.29 4648494 85620
+ std_FusionHeat               1    193.91 4648555 85620
+ mean_ThermalConductivity     1     43.23 4648706 85621
+ std_Valence                  1     12.74 4648736 85621
+ wtd_mean_Valence             1      9.57 4648739 85621
+ wtd_gmean_Valence            1      7.63 4648741 85621
+ mean_atomic_radius           1      1.06 4648748 85621

Step:  AIC=85613.37
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
```

```
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat

                             Df Sum of Sq     RSS   AIC
+ std_FusionHeat              1    7637.6 4638827 85591
+ entropy_FusionHeat          1    3471.5 4642993 85604
+ mean_FusionHeat             1    3125.4 4643339 85605
+ entropy_ThermalConductivity 1    2423.4 4644041 85608
+ wtd_gmean_FusionHeat        1    1996.3 4644468 85609
+ entropy_atomic_radius       1    1771.6 4644693 85610
+ mean_Valence                1    1280.5 4645184 85611
+ gmean_Valence               1    1141.7 4645323 85612
<none>                                   4646465 85613
+ gmean_Density               1     470.7 4645994 85614
+ gmean_fie                   1     372.1 4646093 85614
+ gmean_FusionHeat            1     354.1 4646111 85614
+ wtd_range_atomic_mass       1     349.2 4646115 85614
+ mean_fie                    1     252.5 4646212 85615
+ mean_ThermalConductivity    1     159.8 4646305 85615
+ wtd_mean_fie                1      81.5 4646383 85615
+ wtd_gmean_Valence           1      48.3 4646416 85615
+ std_Valence                 1      25.3 4646439 85615
+ mean_atomic_radius          1       1.0 4646464 85615
+ wtd_mean_Valence            1       0.9 4646464 85615

Step:  AIC=85590.89
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
```

```
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat

                             Df Sum of Sq     RSS   AIC
+ entropy_ThermalConductivity  1   2841.19 4635986 85584
+ entropy_atomic_radius        1   1992.41 4636835 85586
+ wtd_gmean_FusionHeat         1   1685.37 4637142 85587
+ entropy_FusionHeat           1   1646.84 4637180 85588
+ mean_FusionHeat              1    979.29 4637848 85590
+ gmean_Density                1    828.77 4637998 85590
+ mean_Valence                 1    692.15 4638135 85591
<none>                                    4638827 85591
+ gmean_Valence                1    620.17 4638207 85591
+ wtd_gmean_Valence            1    423.61 4638403 85592
+ std_Valence                  1    263.87 4638563 85592
+ gmean_fie                    1    248.89 4638578 85592
+ gmean_FusionHeat             1    234.97 4638592 85592
+ wtd_mean_Valence             1    196.36 4638631 85592
+ mean_fie                     1    157.10 4638670 85592
+ wtd_range_atomic_mass        1    138.55 4638689 85592
+ wtd_mean_fie                 1    104.41 4638723 85593
+ mean_ThermalConductivity     1     74.70 4638752 85593
+ mean_atomic_radius           1     12.91 4638814 85593

Step:  AIC=85583.77
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
```

```
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity

                          Df Sum of Sq     RSS   AIC
+ entropy_FusionHeat       1   2111.25 4633875 85579
+ entropy_atomic_radius    1   1956.02 4634030 85579
+ wtd_gmean_FusionHeat     1   1384.43 4634601 85581
+ mean_Valence             1   1235.66 4634750 85582
+ gmean_Valence            1   1126.66 4634859 85582
+ mean_ThermalConductivity 1   1016.17 4634970 85583
+ gmean_Density            1    922.44 4635063 85583
+ mean_FusionHeat          1    820.90 4635165 85583
<none>                                 4635986 85584
+ wtd_gmean_Valence        1    328.76 4635657 85585
+ wtd_range_atomic_mass    1    200.97 4635785 85585
+ gmean_FusionHeat         1    144.86 4635841 85585
+ std_Valence              1    142.88 4635843 85585
+ wtd_mean_Valence         1    127.39 4635858 85585
+ wtd_mean_fie             1    115.00 4635871 85585
+ gmean_fie                1     52.26 4635934 85586
+ mean_atomic_radius       1     33.56 4635952 85586
+ mean_fie                 1     16.83 4635969 85586

Step:  AIC=85578.99
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
```

```
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat

                           Df Sum of Sq     RSS   AIC
+ mean_FusionHeat           1   2731.12 4631144 85572
+ wtd_gmean_FusionHeat      1   2477.41 4631397 85573
+ entropy_atomic_radius     1   2383.17 4631491 85573
+ mean_ThermalConductivity  1   1524.36 4632350 85576
+ gmean_Density             1   1150.95 4632724 85577
+ gmean_FusionHeat          1   1065.31 4632809 85578
+ mean_Valence              1    960.86 4632914 85578
+ gmean_Valence             1    861.18 4633013 85578
+ wtd_gmean_Valence         1    661.53 4633213 85579
<none>                                  4633875 85579
+ wtd_mean_Valence          1    338.63 4633536 85580
+ std_Valence               1    232.43 4633642 85580
+ wtd_mean_fie              1    228.81 4633646 85580
+ wtd_range_atomic_mass     1    211.50 4633663 85580
+ gmean_fie                 1     31.79 4633843 85581
+ mean_atomic_radius        1     20.59 4633854 85581
+ mean_fie                  1     20.23 4633854 85581

Step:  AIC=85572.21
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
```

```
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat

                           Df Sum of Sq     RSS   AIC
+ entropy_atomic_radius     1   3122.12 4628021 85564
+ wtd_gmean_FusionHeat      1   2269.26 4628874 85567
+ mean_ThermalConductivity  1   1500.17 4629643 85569
+ gmean_Density             1   1042.22 4630101 85571
+ wtd_gmean_Valence         1   1000.14 4630143 85571
+ gmean_FusionHeat          1    690.84 4630453 85572
<none>                                  4631144 85572
+ wtd_mean_Valence          1    607.09 4630536 85572
+ mean_Valence              1    397.26 4630746 85573
+ wtd_range_atomic_mass     1    352.49 4630791 85573
+ gmean_Valence             1    335.31 4630808 85573
+ std_Valence               1    191.53 4630952 85574
+ wtd_mean_fie              1    170.14 4630973 85574
+ gmean_fie                 1    161.85 4630982 85574
+ mean_fie                  1    116.51 4631027 85574
+ mean_atomic_radius        1     28.67 4631115 85574

Step:  AIC=85564.18
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
```

```
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius

                           Df Sum of Sq     RSS   AIC
+ wtd_gmean_FusionHeat      1   2381.43 4625640 85559
+ mean_ThermalConductivity  1   1308.48 4626713 85562
+ gmean_Density             1   1068.18 4626953 85563
+ wtd_gmean_Valence         1    953.76 4627068 85563
+ gmean_FusionHeat          1    781.78 4627240 85564
+ wtd_mean_fie              1    720.16 4627301 85564
<none>                                  4628021 85564
+ wtd_mean_Valence          1    607.55 4627414 85564
+ wtd_range_atomic_mass     1    544.20 4627477 85564
+ mean_Valence              1    400.73 4627621 85565
+ gmean_Valence             1    377.41 4627644 85565
+ std_Valence               1    174.40 4627847 85566
+ mean_fie                  1     84.35 4627937 85566
+ gmean_fie                 1     61.87 4627960 85566
+ mean_atomic_radius        1      3.58 4628018 85566

Step:  AIC=85558.51
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
```

```
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat

                           Df Sum of Sq     RSS   AIC
+ gmean_FusionHeat          1    8637.6 4617002 85533
+ mean_ThermalConductivity  1    1158.3 4624482 85557
+ gmean_Density             1    1041.9 4624598 85557
+ wtd_range_atomic_mass     1     814.8 4624825 85558
+ wtd_gmean_Valence         1     709.7 4624930 85558
+ mean_Valence              1     677.5 4624962 85558
+ gmean_Valence             1     651.0 4624989 85558
<none>                                 4625640 85559
+ wtd_mean_Valence          1     405.8 4625234 85559
+ wtd_mean_fie              1     386.4 4625254 85559
+ std_Valence               1     180.4 4625460 85560
+ mean_fie                  1      54.2 4625586 85560
+ gmean_fie                 1      27.2 4625613 85560
+ mean_atomic_radius        1       0.0 4625640 85561

Step:  AIC=85532.7
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat
```

```
                           Df Sum of Sq     RSS   AIC
+ gmean_Density             1   1861.12 4615141 85529
+ mean_ThermalConductivity  1   1729.01 4615273 85529
+ wtd_range_atomic_mass     1   1070.46 4615932 85531
+ wtd_gmean_Valence         1    905.92 4616096 85532
+ gmean_Valence             1    873.71 4616129 85532
+ mean_Valence              1    836.82 4616166 85532
<none>                                  4617002 85533
+ wtd_mean_Valence          1    551.36 4616451 85533
+ wtd_mean_fie              1    312.08 4616690 85534
+ mean_atomic_radius        1    240.34 4616762 85534
+ mean_fie                  1    197.73 4616805 85534
+ std_Valence               1    175.05 4616827 85534
+ gmean_fie                 1    131.93 4616870 85534

Step:  AIC=85528.69
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density

                           Df Sum of Sq     RSS   AIC
+ mean_ThermalConductivity  1   1765.19 4613376 85525
+ wtd_gmean_Valence         1    927.82 4614213 85528
+ gmean_Valence             1    848.31 4614293 85528
```

```
+ wtd_range_atomic_mass     1    831.86 4614309 85528
+ mean_Valence              1    802.38 4614339 85528
<none>                                  4615141 85529
+ wtd_mean_Valence          1    565.30 4614576 85529
+ mean_atomic_radius        1    308.08 4614833 85530
+ wtd_mean_fie              1    164.28 4614977 85530
+ std_Valence               1    131.02 4615010 85530
+ mean_fie                  1     84.25 4615057 85530
+ gmean_fie                 1     46.10 4615095 85531

Step:  AIC=85525
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity

                        Df Sum of Sq     RSS   AIC
+ gmean_Valence          1   1171.29 4612205 85523
+ mean_Valence           1   1140.35 4612236 85523
+ wtd_range_atomic_mass  1    774.90 4612601 85524
+ wtd_gmean_Valence      1    637.83 4612738 85525
<none>                              4613376 85525
+ mean_atomic_radius     1    443.24 4612933 85526
+ wtd_mean_Valence       1    340.01 4613036 85526
+ wtd_mean_fie           1    126.82 4613249 85527
+ std_Valence            1    125.86 4613250 85527
```

```
+ mean_fie               1     48.55 4613328 85527
+ gmean_fie              1     23.64 4613352 85527

Step:  AIC=85523.22
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity +
    gmean_Valence

                        Df Sum of Sq     RSS   AIC
+ wtd_gmean_Valence      1   10474.3 4601730 85491
+ wtd_mean_Valence       1    8633.0 4603572 85497
+ wtd_range_atomic_mass  1     644.3 4611560 85523
<none>                               4612205 85523
+ mean_atomic_radius     1     514.3 4611690 85524
+ std_Valence            1     115.1 4612090 85525
+ mean_fie               1      78.8 4612126 85525
+ wtd_mean_fie           1      42.0 4612163 85525
+ gmean_fie              1      40.2 4612165 85525
+ mean_Valence           1       2.4 4612202 85525

Step:  AIC=85491.38
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
```

```
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity +
    gmean_Valence + wtd_gmean_Valence

                        Df Sum of Sq     RSS   AIC
+ wtd_mean_Valence       1   1448.16 4600282 85489
+ mean_atomic_radius     1    748.25 4600982 85491
<none>                               4601730 85491
+ wtd_range_atomic_mass  1    526.61 4601204 85492
+ wtd_mean_fie           1    106.83 4601624 85493
+ mean_Valence           1     65.11 4601665 85493
+ mean_fie               1     20.15 4601710 85493
+ std_Valence            1     13.40 4601717 85493
+ gmean_fie              1      2.24 4601728 85493

Step:  AIC=85488.7
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
```

```
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity +
    gmean_Valence + wtd_gmean_Valence + wtd_mean_Valence

                        Df Sum of Sq     RSS   AIC
+ mean_atomic_radius     1    708.08 4599574 85488
+ mean_Valence           1    698.35 4599584 85488
<none>                              4600282 85489
+ wtd_range_atomic_mass  1    524.82 4599757 85489
+ wtd_mean_fie           1    353.27 4599929 85490
+ std_Valence            1    108.67 4600174 85490
+ mean_fie               1      1.47 4600281 85491
+ gmean_fie              1      0.22 4600282 85491

Step:  AIC=85488.41
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
```

```
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity +
    gmean_Valence + wtd_gmean_Valence + wtd_mean_Valence + mean_atomic_radius

                        Df Sum of Sq     RSS   AIC
+ mean_Valence           1    689.04 4598885 85488
<none>                               4599574 85488
+ wtd_range_atomic_mass  1    455.33 4599119 85489
+ wtd_mean_fie           1    380.13 4599194 85489
+ std_Valence            1    112.77 4599461 85490
+ gmean_fie              1     30.65 4599544 85490
+ mean_fie               1      9.27 4599565 85490

Step:  AIC=85488.18
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity +
    gmean_Valence + wtd_gmean_Valence + wtd_mean_Valence + mean_atomic_radius +
    mean_Valence

                        Df Sum of Sq     RSS   AIC
```

```
+ std_Valence            1   1038.51 4597847 85487
<none>                                4598885 85488
+ wtd_range_atomic_mass  1    471.09 4598414 85489
+ wtd_mean_fie           1    290.27 4598595 85489
+ gmean_fie              1      9.97 4598875 85490
+ mean_fie               1      0.08 4598885 85490

Step:  AIC=85486.81
critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass
+
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity
+
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity +
    gmean_Valence + wtd_gmean_Valence + wtd_mean_Valence + mean_atomic_radius +
    mean_Valence + std_Valence

                        Df Sum of Sq     RSS   AIC
<none>                                4597847 85487
+ wtd_range_atomic_mass  1    442.28 4597404 85487
+ wtd_mean_fie           1    261.96 4597585 85488
+ gmean_fie              1      6.66 4597840 85489
+ mean_fie               1      0.63 4597846 85489

Call:
lm(formula = critical_temp ~ wtd_std_ThermalConductivity + gmean_ElectronAffinity +
    range_atomic_radius + std_atomic_radius + entropy_ElectronAffinity +
    wtd_gmean_ElectronAffinity + wtd_std_Valence + wtd_entropy_atomic_mass +
```

```
    wtd_entropy_Density + range_atomic_mass + wtd_std_atomic_mass +
    wtd_entropy_ThermalConductivity + range_Density + range_ThermalConductivity +
    gmean_ThermalConductivity + wtd_entropy_ElectronAffinity +
    wtd_mean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    wtd_entropy_FusionHeat + wtd_range_Valence + wtd_std_ElectronAffinity +
    wtd_mean_ElectronAffinity + std_ElectronAffinity + range_ElectronAffinity +
    wtd_range_ThermalConductivity + wtd_std_atomic_radius + entropy_atomic_mass +
    wtd_std_FusionHeat + wtd_entropy_fie + range_Valence + wtd_entropy_Valence +
    wtd_range_FusionHeat + std_ThermalConductivity + wtd_range_ElectronAffinity +
    wtd_range_fie + mean_ElectronAffinity + wtd_range_Density +
    std_atomic_mass + mean_Density + mean_atomic_mass + wtd_gmean_Density +
    wtd_mean_atomic_mass + std_Density + wtd_std_Density + entropy_Density +
    gmean_atomic_mass + wtd_mean_atomic_radius + wtd_gmean_atomic_radius +
    wtd_std_fie + wtd_range_atomic_radius + gmean_atomic_radius +
    wtd_entropy_atomic_radius + wtd_mean_FusionHeat + wtd_gmean_fie +
    wtd_mean_Density + entropy_Valence + entropy_fie + range_fie +
    std_fie + number_of_elements + wtd_gmean_atomic_mass + range_FusionHeat +
    std_FusionHeat + entropy_ThermalConductivity + entropy_FusionHeat +
    mean_FusionHeat + entropy_atomic_radius + wtd_gmean_FusionHeat +
    gmean_FusionHeat + gmean_Density + mean_ThermalConductivity +
    gmean_Valence + wtd_gmean_Valence + wtd_mean_Valence + mean_atomic_radius +
    mean_Valence + std_Valence, data = train)

Residuals:
    Min      1Q  Median      3Q     Max
-84.560  -9.389   0.529  10.877 169.768

Coefficients:
                                 Estimate Std. Error t value Pr(>|t|)
(Intercept)                    -2.676e+01  5.537e+00  -4.833 1.36e-06 ***
wtd_std_ThermalConductivity    -2.235e-02  2.694e-02  -0.830 0.406824
gmean_ElectronAffinity          1.442e-01  4.777e-02   3.018 0.002548 **
range_atomic_radius             2.083e-01  2.653e-02   7.851 4.40e-15 ***
std_atomic_radius              -4.889e-01  1.161e-01  -4.210 2.56e-05 ***
entropy_ElectronAffinity        5.231e+00  3.057e+00   1.711 0.087106 .
wtd_gmean_ElectronAffinity     -5.430e-01  5.315e-02 -10.216  < 2e-16 ***
wtd_std_Valence                -2.645e+01  2.284e+00 -11.581  < 2e-16 ***
wtd_entropy_atomic_mass         4.199e+00  3.932e+00   1.068 0.285618
wtd_entropy_Density            -1.865e+01  3.042e+00  -6.132 8.87e-10 ***
range_atomic_mass               2.171e-01  1.965e-02  11.050  < 2e-16 ***
wtd_std_atomic_mass             9.115e-02  6.575e-02   1.386 0.165668
wtd_entropy_ThermalConductivity 2.201e+00  1.900e+00   1.158 0.246931
range_Density                  -1.673e-03  2.566e-04  -6.518 7.35e-11 ***
range_ThermalConductivity      -9.563e-02  1.581e-02  -6.048 1.50e-09 ***
gmean_ThermalConductivity      -5.843e-02  2.765e-02  -2.114 0.034566 *
wtd_entropy_ElectronAffinity   -2.397e+01  2.627e+00  -9.125  < 2e-16 ***
wtd_mean_ThermalConductivity    5.442e-01  3.235e-02  16.824  < 2e-16 ***
wtd_gmean_ThermalConductivity  -3.436e-01  3.124e-02 -10.999  < 2e-16 ***
```

```
wtd_entropy_FusionHeat           2.573e+01  2.287e+00  11.251  < 2e-16 ***
wtd_range_Valence               -1.061e+00  7.575e-01  -1.401 0.161292
wtd_std_ElectronAffinity        -5.245e-01  4.688e-02 -11.188  < 2e-16 ***
wtd_mean_ElectronAffinity        4.974e-01  5.984e-02   8.311  < 2e-16 ***
std_ElectronAffinity             1.250e+00  6.914e-02  18.073  < 2e-16 ***
range_ElectronAffinity          -3.813e-01  2.042e-02 -18.669  < 2e-16 ***
wtd_range_ThermalConductivity   -2.266e-01  1.926e-02 -11.769  < 2e-16 ***
wtd_std_atomic_radius           -1.970e-01  1.022e-01  -1.927 0.053997 .
entropy_atomic_mass             -3.695e+01  5.292e+00  -6.981 3.06e-12 ***
wtd_std_FusionHeat               6.915e-01  1.818e-01   3.803 0.000144 ***
wtd_entropy_fie                  4.999e+01  5.469e+00   9.141  < 2e-16 ***
range_Valence                    5.758e+00  8.777e-01   6.560 5.56e-11 ***
wtd_entropy_Valence             -6.861e+01  6.575e+00 -10.435  < 2e-16 ***
wtd_range_FusionHeat             6.221e-01  7.960e-02   7.816 5.83e-15 ***
std_ThermalConductivity          3.027e-01  4.911e-02   6.164 7.27e-10 ***
wtd_range_ElectronAffinity      -1.570e-01  2.492e-02  -6.300 3.06e-10 ***
wtd_range_fie                    2.468e-02  4.288e-03   5.756 8.78e-09 ***
mean_ElectronAffinity           -7.839e-02  5.368e-02  -1.460 0.144246
wtd_range_Density                2.875e-04  2.353e-04   1.222 0.221799
std_atomic_mass                 -5.679e-01  7.497e-02  -7.574 3.82e-14 ***
mean_Density                    -5.049e-03  5.885e-04  -8.579  < 2e-16 ***
mean_atomic_mass                 8.004e-01  9.896e-02   8.088 6.55e-16 ***
wtd_gmean_Density                1.993e-03  6.774e-04   2.942 0.003263 **
wtd_mean_atomic_mass            -8.058e-01  1.227e-01  -6.568 5.27e-11 ***
std_Density                      6.474e-03  8.298e-04   7.801 6.53e-15 ***
wtd_std_Density                 -1.803e-03  6.131e-04  -2.940 0.003282 **
entropy_Density                  1.649e+01  4.007e+00   4.115 3.89e-05 ***
gmean_atomic_mass               -4.542e-01  9.749e-02  -4.659 3.20e-06 ***
wtd_mean_atomic_radius           2.829e+00  2.686e-01  10.532  < 2e-16 ***
wtd_gmean_atomic_radius         -2.430e+00  2.627e-01  -9.249  < 2e-16 ***
wtd_std_fie                     -7.371e-02  1.249e-02  -5.903 3.66e-09 ***
wtd_range_atomic_radius         -8.525e-02  1.772e-02  -4.810 1.53e-06 ***
gmean_atomic_radius             -1.880e-02  2.079e-01  -0.090 0.927932
wtd_entropy_atomic_radius        4.048e+01  6.189e+00   6.541 6.32e-11 ***
wtd_mean_FusionHeat             -1.860e+00  2.256e-01  -8.243  < 2e-16 ***
wtd_gmean_fie                    3.083e-02  4.892e-03   6.303 3.00e-10 ***
wtd_mean_Density                -2.185e-04  7.040e-04  -0.310 0.756318
entropy_Valence                  7.488e+01  1.404e+01   5.333 9.81e-08 ***
entropy_fie                     -1.116e+02  2.119e+01  -5.267 1.41e-07 ***
range_fie                        6.844e-02  7.756e-03   8.825  < 2e-16 ***
std_fie                         -1.518e-01  2.027e-02  -7.489 7.32e-14 ***
number_of_elements              -2.787e+00  8.849e-01  -3.150 0.001637 **
wtd_gmean_atomic_mass            5.632e-01  1.175e-01   4.794 1.65e-06 ***
range_FusionHeat                -4.088e-01  7.935e-02  -5.153 2.60e-07 ***
std_FusionHeat                  -3.911e-01  3.116e-01  -1.255 0.209415
entropy_ThermalConductivity      1.118e+01  2.352e+00   4.752 2.04e-06 ***
entropy_FusionHeat              -1.947e+01  3.224e+00  -6.041 1.57e-09 ***
mean_FusionHeat                  1.593e+00  2.241e-01   7.111 1.21e-12 ***
```

```
entropy_atomic_radius             6.792e+01  1.885e+01   3.603 0.000315 ***
wtd_gmean_FusionHeat              1.510e+00  2.097e-01   7.204 6.15e-13 ***
gmean_FusionHeat                 -1.405e+00  2.047e-01  -6.863 7.02e-12 ***
gmean_Density                     1.546e-03  5.501e-04   2.811 0.004944 **
mean_ThermalConductivity         -6.503e-02  2.918e-02  -2.228 0.025867 *
gmean_Valence                     2.060e+01  6.791e+00   3.034 0.002419 **
wtd_gmean_Valence                -3.123e+01  8.178e+00  -3.819 0.000134 ***
wtd_mean_Valence                  2.743e+01  8.723e+00   3.145 0.001665 **
mean_atomic_radius               -3.104e-01  2.059e-01  -1.508 0.131644
mean_Valence                     -1.643e+01  7.205e+00  -2.280 0.022602 *
std_Valence                       5.361e+00  2.932e+00   1.829 0.067462 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.62 on 14806 degrees of freedom
Multiple R-squared:  0.7368,Adjusted R-squared:  0.7354
F-statistic: 538.2 on 77 and 14806 DF,  p-value: < 2.2e-16
```

[47]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.step.forward.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 77 predictors is been used"
```

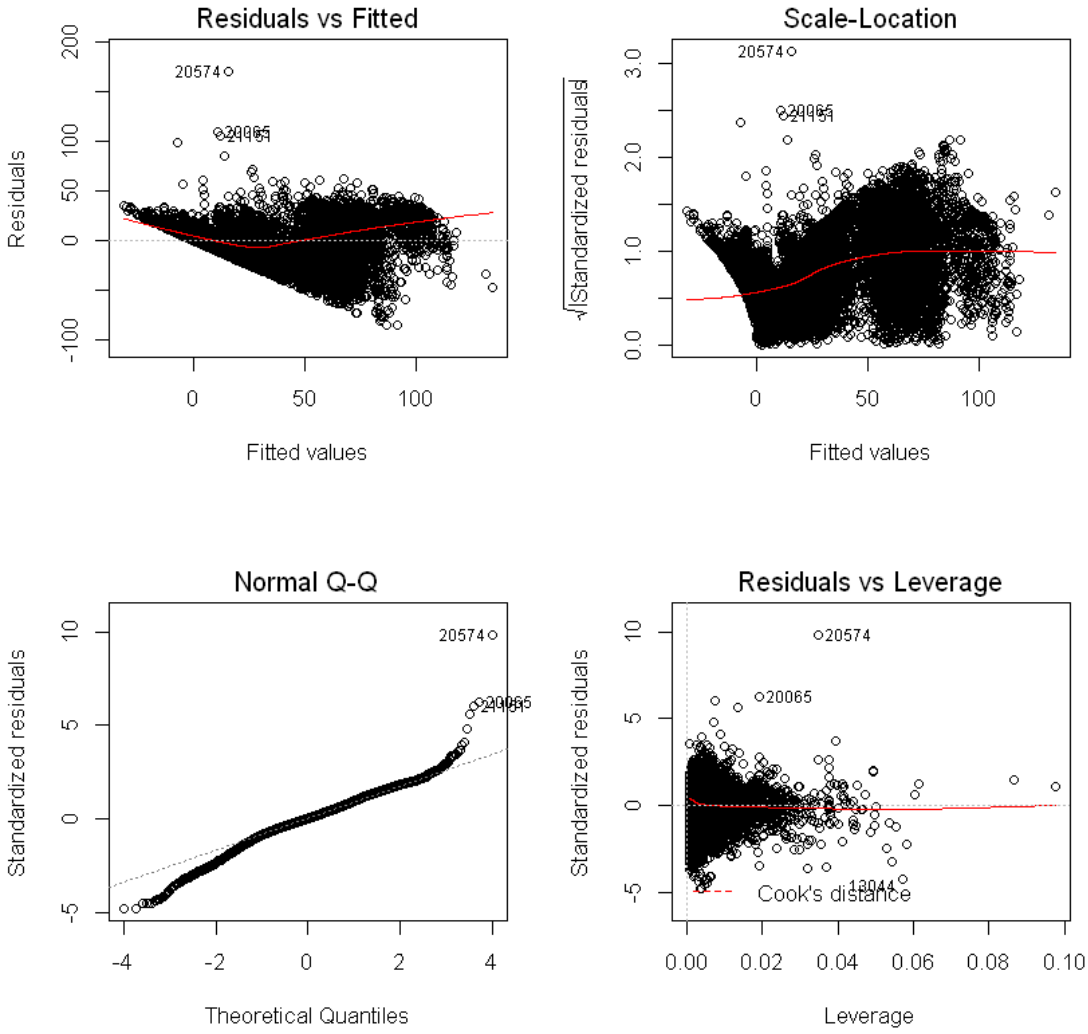
[48]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.all.summary$adj.r.
 ↪squared,4)))
print(paste("Step Forward Data - Adjusted R-Square:",round(fit.step.forward.
 ↪summary$adj.r.squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7355"
[1] "Step Forward Data - Adjusted R-Square: 0.7354"
```

Here we can see that the adjusted R-square is decreased but only for a small amount which indicates that it might be a better model compared to original model(including all predicates) as this model is comparitively less complex

Lets Check the various Residuals plot

[49]:
```
par(mfcol=c(2,2))
plot(fit.step.forward)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if

residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.7 Perform F-tests by comparing the two models using the anova() function

[50]:
```
anova(fit.all, fit.step.forward)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14806	4597847	-4	-2948.009	2.374178	0.04986433

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are more correlated as p value is less than 0.05. we can also see that in the new fit the no of predictors is less compared to the original which makes it less complex. Also we can see that there is only slight increase in RSS compared to the original fit. So due to all these factors the new model looks better than the all predictors model

4.1.8 Generating a linear Fit using backward step function

[51]:
```
fit.step.backward = step(lm(critical_temp~. , data = train),direction =␣
 ↪"backward")
fit.step.backward.summary <-summary(fit.step.backward)
fit.step.backward.summary
```

```
Start:  AIC=85485.27
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + wtd_std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + gmean_atomic_radius + wtd_gmean_atomic_radius +
    entropy_atomic_radius + wtd_entropy_atomic_radius + range_atomic_radius +
```

```
    wtd_range_atomic_radius + std_atomic_radius + wtd_std_atomic_radius +
    mean_Density + wtd_mean_Density + gmean_Density + wtd_gmean_Density +
    entropy_Density + wtd_entropy_Density + range_Density + wtd_range_Density +
    std_Density + wtd_std_Density + mean_ElectronAffinity +
wtd_mean_ElectronAffinity +
    gmean_ElectronAffinity + wtd_gmean_ElectronAffinity +
entropy_ElectronAffinity +
    wtd_entropy_ElectronAffinity + range_ElectronAffinity +
wtd_range_ElectronAffinity +
    std_ElectronAffinity + wtd_std_ElectronAffinity + mean_FusionHeat +
    wtd_mean_FusionHeat + gmean_FusionHeat + wtd_gmean_FusionHeat +
    entropy_FusionHeat + wtd_entropy_FusionHeat + range_FusionHeat +
    wtd_range_FusionHeat + std_FusionHeat + wtd_std_FusionHeat +
    mean_ThermalConductivity + wtd_mean_ThermalConductivity +
    gmean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    entropy_ThermalConductivity + wtd_entropy_ThermalConductivity +
    range_ThermalConductivity + wtd_range_ThermalConductivity +
    std_ThermalConductivity + wtd_std_ThermalConductivity + mean_Valence +
    wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence + entropy_Valence +
    wtd_entropy_Valence + range_Valence + wtd_range_Valence +
    std_Valence + wtd_std_Valence

                                Df Sum of Sq     RSS   AIC
- wtd_range_Density              1         2 4594900 85483
- wtd_mean_Density               1         8 4594906 85483
- gmean_atomic_radius            1        76 4594975 85484
- wtd_std_fie                    1       146 4595045 85484
- wtd_std_ThermalConductivity    1       195 4595094 85484
- wtd_range_Valence              1       443 4595341 85485
- wtd_entropy_ThermalConductivity 1      499 4595398 85485
- mean_ElectronAffinity          1       525 4595424 85485
- wtd_range_atomic_mass          1       586 4595485 85485
<none>                                     4594899 85485
- wtd_std_atomic_mass            1       668 4595567 85485
- std_FusionHeat                 1       682 4595580 85485
- wtd_entropy_atomic_mass        1       774 4595673 85486
- entropy_ElectronAffinity       1       998 4595897 85486
- mean_ThermalConductivity       1      1076 4595975 85487
- std_Valence                    1      1296 4596194 85487
- mean_atomic_radius             1      1323 4596222 85488
- gmean_Density                  1      1365 4596263 85488
- gmean_ThermalConductivity      1      1664 4596562 85489
- wtd_std_atomic_radius          1      1667 4596565 85489
- mean_Valence                   1      1768 4596666 85489
- wtd_mean_fie                   1      2097 4596995 85490
- gmean_fie                      1      2205 4597104 85490
- mean_fie                       1      2208 4597106 85490
- gmean_ElectronAffinity         1      2412 4597311 85491
```

```
- wtd_std_Density                1      2546 4597444 85492
- wtd_gmean_fie                  1      2660 4597559 85492
- gmean_Valence                  1      3041 4597940 85493
- wtd_mean_Valence               1      3289 4598188 85494
- wtd_gmean_Density              1      3537 4598436 85495
- number_of_elements             1      3652 4598551 85495
- wtd_std_FusionHeat             1      3934 4598832 85496
- std_atomic_radius              1      4466 4599365 85498
- entropy_Density                1      4849 4599748 85499
- wtd_gmean_Valence              1      4859 4599758 85499
- entropy_atomic_radius          1      4867 4599765 85499
- entropy_ThermalConductivity    1      6061 4600960 85503
- gmean_atomic_mass              1      6244 4601143 85503
- wtd_gmean_atomic_mass          1      6722 4601621 85505
- range_FusionHeat               1      6796 4601695 85505
- wtd_range_atomic_radius        1      7957 4602856 85509
- entropy_fie                    1      8890 4603789 85512
- entropy_Valence                1      9058 4603957 85513
- wtd_range_fie                  1      9405 4604303 85514
- entropy_FusionHeat             1      9543 4604442 85514
- range_ThermalConductivity      1     11145 4606044 85519
- std_ThermalConductivity        1     11374 4606272 85520
- wtd_entropy_atomic_radius      1     11703 4606601 85521
- wtd_entropy_Density            1     11950 4606849 85522
- wtd_range_ElectronAffinity     1     12767 4607666 85525
- range_Valence                  1     13024 4607922 85525
- wtd_mean_atomic_mass           1     13951 4608850 85528
- range_Density                  1     14161 4609059 85529
- gmean_FusionHeat               1     15101 4609999 85532
- entropy_atomic_mass            1     15719 4610617 85534
- wtd_gmean_FusionHeat           1     15981 4610880 85535
- mean_FusionHeat                1     16798 4611697 85538
- std_fie                        1     17640 4612539 85540
- std_atomic_mass                1     18477 4613376 85543
- range_atomic_radius            1     19134 4614032 85545
- std_Density                    1     19513 4614412 85546
- wtd_mean_ElectronAffinity      1     20110 4615008 85548
- wtd_range_FusionHeat           1     20406 4615304 85549
- mean_atomic_mass               1     20671 4615569 85550
- wtd_entropy_fie                1     21530 4616428 85553
- wtd_mean_FusionHeat            1     21532 4616430 85553
- mean_Density                   1     21539 4616437 85553
- range_fie                      1     23362 4618261 85559
- wtd_entropy_ElectronAffinity   1     26586 4621485 85569
- wtd_gmean_atomic_radius        1     27587 4622486 85572
- wtd_gmean_ElectronAffinity     1     30164 4625063 85581
- wtd_entropy_Valence            1     31288 4626186 85584
- wtd_gmean_ThermalConductivity  1     33878 4628777 85593
```

```
- wtd_mean_atomic_radius           1     35204 4630102 85597
- range_atomic_mass                1     37685 4632584 85605
- wtd_entropy_FusionHeat           1     38483 4633382 85607
- wtd_std_ElectronAffinity         1     38586 4633485 85608
- wtd_range_ThermalConductivity    1     39863 4634762 85612
- wtd_std_Valence                  1     42746 4637644 85621
- wtd_mean_ThermalConductivity     1     77111 4672009 85731
- std_ElectronAffinity             1     98552 4693450 85799
- range_ElectronAffinity           1    101718 4696617 85809

Step:  AIC=85483.27
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + wtd_std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + gmean_atomic_radius + wtd_gmean_atomic_radius +
    entropy_atomic_radius + wtd_entropy_atomic_radius + range_atomic_radius +
    wtd_range_atomic_radius + std_atomic_radius + wtd_std_atomic_radius +
    mean_Density + wtd_mean_Density + gmean_Density + wtd_gmean_Density +
    entropy_Density + wtd_entropy_Density + range_Density + std_Density +
    wtd_std_Density + mean_ElectronAffinity + wtd_mean_ElectronAffinity +
    gmean_ElectronAffinity + wtd_gmean_ElectronAffinity +
entropy_ElectronAffinity +
    wtd_entropy_ElectronAffinity + range_ElectronAffinity +
wtd_range_ElectronAffinity +
    std_ElectronAffinity + wtd_std_ElectronAffinity + mean_FusionHeat +
    wtd_mean_FusionHeat + gmean_FusionHeat + wtd_gmean_FusionHeat +
    entropy_FusionHeat + wtd_entropy_FusionHeat + range_FusionHeat +
    wtd_range_FusionHeat + std_FusionHeat + wtd_std_FusionHeat +
    mean_ThermalConductivity + wtd_mean_ThermalConductivity +
    gmean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    entropy_ThermalConductivity + wtd_entropy_ThermalConductivity +
    range_ThermalConductivity + wtd_range_ThermalConductivity +
    std_ThermalConductivity + wtd_std_ThermalConductivity + mean_Valence +
    wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence + entropy_Valence +
    wtd_entropy_Valence + range_Valence + wtd_range_Valence +
    std_Valence + wtd_std_Valence

                                  Df Sum of Sq     RSS   AIC
- wtd_mean_Density                 1        11 4594911 85481
- gmean_atomic_radius              1        77 4594978 85482
- wtd_std_fie                      1       148 4595048 85482
- wtd_std_ThermalConductivity      1       196 4595096 85482
- wtd_range_Valence                1       492 4595393 85483
- wtd_entropy_ThermalConductivity  1       505 4595406 85483
- mean_ElectronAffinity            1       524 4595425 85483
```

```
<none>                                  4594900 85483
- wtd_std_atomic_mass             1       677 4595577 85483
- std_FusionHeat                  1       686 4595586 85483
- wtd_entropy_atomic_mass         1       805 4595705 85484
- wtd_range_atomic_mass           1       953 4595853 85484
- entropy_ElectronAffinity        1      1002 4595902 85485
- mean_ThermalConductivity        1      1075 4595975 85485
- std_Valence                     1      1294 4596194 85485
- mean_atomic_radius              1      1330 4596230 85486
- gmean_Density                   1      1443 4596343 85486
- gmean_ThermalConductivity       1      1678 4596578 85487
- wtd_std_atomic_radius           1      1691 4596592 85487
- mean_Valence                    1      1767 4596667 85487
- wtd_mean_fie                    1      2098 4596998 85488
- gmean_fie                       1      2208 4597108 85488
- mean_fie                        1      2213 4597113 85488
- gmean_ElectronAffinity          1      2411 4597311 85489
- wtd_std_Density                 1      2552 4597452 85490
- wtd_gmean_fie                   1      2662 4597562 85490
- gmean_Valence                   1      3040 4597941 85491
- wtd_mean_Valence                1      3292 4598193 85492
- wtd_gmean_Density               1      3590 4598490 85493
- number_of_elements              1      3652 4598553 85493
- wtd_std_FusionHeat              1      3961 4598861 85494
- std_atomic_radius               1      4479 4599379 85496
- entropy_atomic_radius           1      4866 4599766 85497
- wtd_gmean_Valence               1      4871 4599771 85497
- entropy_Density                 1      5010 4599910 85497
- entropy_ThermalConductivity     1      6066 4600967 85501
- gmean_atomic_mass               1      6308 4601208 85502
- wtd_gmean_atomic_mass           1      6807 4601707 85503
- range_FusionHeat                1      6887 4601788 85504
- wtd_range_atomic_radius         1      7986 4602886 85507
- entropy_fie                     1      8914 4603815 85510
- entropy_Valence                 1      9075 4603975 85511
- wtd_range_fie                   1      9454 4604354 85512
- entropy_FusionHeat              1      9665 4604565 85513
- range_ThermalConductivity       1     11253 4606153 85518
- std_ThermalConductivity         1     11374 4606275 85518
- wtd_entropy_atomic_radius       1     11743 4606644 85519
- wtd_range_ElectronAffinity      1     12792 4607692 85523
- range_Valence                   1     13022 4607923 85523
- wtd_mean_atomic_mass            1     13959 4608859 85526
- wtd_entropy_Density             1     14020 4608920 85527
- range_Density                   1     14175 4609075 85527
- gmean_FusionHeat                1     15099 4609999 85530
- entropy_atomic_mass             1     15791 4610691 85532
- wtd_gmean_FusionHeat            1     16011 4610911 85533
```

```
- mean_FusionHeat                  1     16872 4611773 85536
- std_fie                          1     17712 4612612 85539
- std_atomic_mass                  1     18477 4613378 85541
- range_atomic_radius              1     19136 4614037 85543
- std_Density                      1     19743 4614643 85545
- wtd_mean_ElectronAffinity        1     20130 4615030 85546
- mean_atomic_mass                 1     20670 4615570 85548
- wtd_range_FusionHeat             1     21243 4616143 85550
- wtd_mean_FusionHeat              1     21825 4616725 85552
- mean_Density                     1     21832 4616733 85552
- wtd_entropy_fie                  1     21919 4616819 85552
- range_fie                        1     23366 4618266 85557
- wtd_entropy_ElectronAffinity     1     26812 4621712 85568
- wtd_gmean_atomic_radius          1     27664 4622565 85571
- wtd_gmean_ElectronAffinity       1     30216 4625116 85579
- wtd_entropy_Valence              1     32169 4627069 85585
- wtd_gmean_ThermalConductivity    1     33987 4628887 85591
- wtd_mean_atomic_radius           1     35274 4630174 85595
- range_atomic_mass                1     37684 4632584 85603
- wtd_std_ElectronAffinity         1     38600 4633500 85606
- wtd_entropy_FusionHeat           1     38788 4633689 85606
- wtd_range_ThermalConductivity    1     40817 4635717 85613
- wtd_std_Valence                  1     42859 4637759 85619
- wtd_mean_ThermalConductivity     1     77133 4672033 85729
- std_ElectronAffinity             1     98798 4693698 85798
- range_ElectronAffinity           1    101808 4696708 85807

Step:  AIC=85481.31
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + wtd_std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + gmean_atomic_radius + wtd_gmean_atomic_radius +
    entropy_atomic_radius + wtd_entropy_atomic_radius + range_atomic_radius +
    wtd_range_atomic_radius + std_atomic_radius + wtd_std_atomic_radius +
    mean_Density + gmean_Density + wtd_gmean_Density + entropy_Density +
    wtd_entropy_Density + range_Density + std_Density + wtd_std_Density +
    mean_ElectronAffinity + wtd_mean_ElectronAffinity + gmean_ElectronAffinity +
    wtd_gmean_ElectronAffinity + entropy_ElectronAffinity +
wtd_entropy_ElectronAffinity +
    range_ElectronAffinity + wtd_range_ElectronAffinity + std_ElectronAffinity +
    wtd_std_ElectronAffinity + mean_FusionHeat + wtd_mean_FusionHeat +
    gmean_FusionHeat + wtd_gmean_FusionHeat + entropy_FusionHeat +
    wtd_entropy_FusionHeat + range_FusionHeat + wtd_range_FusionHeat +
    std_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
```

```
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    wtd_std_ThermalConductivity + mean_Valence + wtd_mean_Valence +
    gmean_Valence + wtd_gmean_Valence + entropy_Valence + wtd_entropy_Valence +
    range_Valence + wtd_range_Valence + std_Valence + wtd_std_Valence

                                  Df Sum of Sq     RSS   AIC
- gmean_atomic_radius              1        80 4594991 85480
- wtd_std_fie                      1       172 4595083 85480
- wtd_std_ThermalConductivity      1       189 4595099 85480
- wtd_entropy_ThermalConductivity  1       500 4595411 85481
- wtd_range_Valence                1       513 4595424 85481
- mean_ElectronAffinity            1       519 4595430 85481
<none>                                       4594911 85481
- std_FusionHeat                   1       689 4595600 85482
- wtd_std_atomic_mass              1       770 4595680 85482
- wtd_entropy_atomic_mass          1       797 4595708 85482
- wtd_range_atomic_mass            1       954 4595865 85482
- entropy_ElectronAffinity         1      1005 4595916 85483
- mean_ThermalConductivity         1      1069 4595980 85483
- mean_atomic_radius               1      1347 4596257 85484
- std_Valence                      1      1347 4596258 85484
- wtd_std_atomic_radius            1      1681 4596592 85485
- gmean_ThermalConductivity        1      1727 4596638 85485
- mean_Valence                     1      1815 4596726 85485
- wtd_mean_fie                     1      2097 4597008 85486
- gmean_fie                        1      2211 4597122 85486
- mean_fie                         1      2215 4597126 85486
- gmean_ElectronAffinity           1      2401 4597312 85487
- wtd_gmean_fie                    1      2666 4597577 85488
- gmean_Density                    1      2699 4597610 85488
- gmean_Valence                    1      3131 4598042 85489
- wtd_mean_Valence                 1      3337 4598248 85490
- number_of_elements               1      3790 4598701 85492
- wtd_std_Density                  1      3814 4598725 85492
- wtd_std_FusionHeat               1      4137 4599048 85493
- std_atomic_radius                1      4495 4599406 85494
- entropy_atomic_radius            1      4859 4599770 85495
- wtd_gmean_Valence                1      4947 4599858 85495
- entropy_Density                  1      5063 4599974 85496
- entropy_ThermalConductivity      1      6099 4601010 85499
- gmean_atomic_mass                1      6657 4601567 85501
- range_FusionHeat                 1      6928 4601839 85502
- wtd_gmean_atomic_mass            1      7732 4602643 85504
- wtd_range_atomic_radius          1      8018 4602929 85505
- entropy_fie                      1      9022 4603933 85509
- entropy_Valence                  1      9180 4604091 85509
```

```
- entropy_FusionHeat               1      9685 4604596 85511
- wtd_range_fie                    1      9704 4604615 85511
- range_ThermalConductivity        1     11260 4606171 85516
- std_ThermalConductivity          1     11366 4606277 85516
- wtd_entropy_atomic_radius        1     11827 4606738 85518
- wtd_range_ElectronAffinity       1     12814 4607725 85521
- range_Valence                    1     13058 4607969 85522
- wtd_entropy_Density              1     14026 4608937 85525
- range_Density                    1     14165 4609076 85525
- wtd_gmean_Density                1     14819 4609730 85527
- gmean_FusionHeat                 1     15220 4610131 85529
- entropy_atomic_mass              1     15797 4610708 85530
- wtd_mean_atomic_mass             1     16533 4611444 85533
- wtd_gmean_FusionHeat             1     16679 4611590 85533
- mean_FusionHeat                  1     16994 4611904 85534
- std_fie                          1     17730 4612641 85537
- std_atomic_mass                  1     19006 4613917 85541
- range_atomic_radius              1     19132 4614043 85541
- wtd_mean_ElectronAffinity        1     20120 4615031 85544
- wtd_range_FusionHeat             1     21234 4616145 85548
- std_Density                      1     21685 4616596 85549
- wtd_entropy_fie                  1     21924 4616835 85550
- wtd_mean_FusionHeat              1     22621 4617532 85552
- mean_atomic_mass                 1     22656 4617567 85553
- range_fie                        1     23502 4618413 85555
- wtd_entropy_ElectronAffinity     1     26840 4621751 85566
- wtd_gmean_atomic_radius          1     27710 4622621 85569
- wtd_gmean_ElectronAffinity       1     30220 4625131 85577
- wtd_entropy_Valence              1     32281 4627192 85584
- wtd_gmean_ThermalConductivity    1     34812 4629722 85592
- wtd_mean_atomic_radius           1     35306 4630217 85593
- range_atomic_mass                1     37684 4632595 85601
- wtd_entropy_FusionHeat           1     39041 4633951 85605
- wtd_std_ElectronAffinity         1     39883 4634794 85608
- wtd_range_ThermalConductivity    1     41964 4636875 85615
- wtd_std_Valence                  1     43865 4638776 85621
- mean_Density                     1     44759 4639670 85624
- wtd_mean_ThermalConductivity     1     77707 4672618 85729
- std_ElectronAffinity             1     98827 4693738 85796
- range_ElectronAffinity           1    103278 4698189 85810

Step:  AIC=85479.57
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + wtd_std_fie + mean_atomic_radius +
```

```
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + mean_ElectronAffinity +
    wtd_mean_ElectronAffinity + gmean_ElectronAffinity +
wtd_gmean_ElectronAffinity +
    entropy_ElectronAffinity + wtd_entropy_ElectronAffinity +
    range_ElectronAffinity + wtd_range_ElectronAffinity + std_ElectronAffinity +
    wtd_std_ElectronAffinity + mean_FusionHeat + wtd_mean_FusionHeat +
    gmean_FusionHeat + wtd_gmean_FusionHeat + entropy_FusionHeat +
    wtd_entropy_FusionHeat + range_FusionHeat + wtd_range_FusionHeat +
    std_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    wtd_std_ThermalConductivity + mean_Valence + wtd_mean_Valence +
    gmean_Valence + wtd_gmean_Valence + entropy_Valence + wtd_entropy_Valence +
    range_Valence + wtd_range_Valence + std_Valence + wtd_std_Valence

                                Df Sum of Sq     RSS   AIC
- wtd_std_ThermalConductivity    1       171 4595161 85478
- wtd_std_fie                    1       171 4595162 85478
- wtd_range_Valence              1       487 4595478 85479
- wtd_entropy_ThermalConductivity 1      489 4595480 85479
- mean_ElectronAffinity          1       576 4595567 85479
<none>                                       4594991 85480
- std_FusionHeat                 1       637 4595628 85480
- wtd_std_atomic_mass            1       706 4595697 85480
- wtd_entropy_atomic_mass        1       794 4595785 85480
- entropy_ElectronAffinity       1       983 4595974 85481
- wtd_range_atomic_mass          1       990 4595981 85481
- mean_ThermalConductivity       1      1036 4596027 85481
- std_Valence                    1      1325 4596316 85482
- mean_Valence                   1      1797 4596788 85483
- gmean_ThermalConductivity      1      1821 4596812 85483
- wtd_mean_fie                   1      2017 4597008 85484
- gmean_fie                      1      2144 4597135 85485
- mean_fie                       1      2145 4597135 85485
- wtd_std_atomic_radius          1      2286 4597276 85485
- gmean_ElectronAffinity         1      2524 4597514 85486
- wtd_gmean_fie                  1      2590 4597581 85486
- gmean_Density                  1      2757 4597748 85486
- gmean_Valence                  1      3101 4598092 85488
- wtd_mean_Valence               1      3324 4598315 85488
- wtd_std_Density                1      3737 4598728 85490
- number_of_elements             1      3773 4598764 85490
```

```
- wtd_std_FusionHeat               1      4057 4599048 85491
- entropy_atomic_radius            1      4828 4599819 85493
- wtd_gmean_Valence                1      4923 4599914 85494
- entropy_Density                  1      5029 4600020 85494
- entropy_ThermalConductivity      1      6128 4601119 85497
- gmean_atomic_mass                1      6613 4601604 85499
- range_FusionHeat                 1      7092 4602083 85501
- wtd_gmean_atomic_mass            1      7672 4602663 85502
- wtd_range_atomic_radius          1      7995 4602986 85503
- entropy_fie                      1      8942 4603933 85507
- entropy_Valence                  1      9101 4604092 85507
- wtd_range_fie                    1      9625 4604616 85509
- entropy_FusionHeat               1      9655 4604646 85509
- std_atomic_radius                1     10085 4605076 85510
- range_ThermalConductivity        1     11351 4606342 85514
- std_ThermalConductivity          1     11354 4606345 85514
- wtd_entropy_atomic_radius        1     11772 4606763 85516
- wtd_range_ElectronAffinity       1     13082 4608073 85520
- range_Valence                    1     13092 4608083 85520
- wtd_entropy_Density              1     14031 4609022 85523
- range_Density                    1     14282 4609273 85524
- wtd_gmean_Density                1     14830 4609821 85526
- gmean_FusionHeat                 1     15271 4610262 85527
- entropy_atomic_mass              1     15864 4610855 85529
- wtd_mean_atomic_mass             1     16528 4611519 85531
- wtd_gmean_FusionHeat             1     16674 4611665 85531
- mean_FusionHeat                  1     17069 4612060 85533
- std_fie                          1     17688 4612679 85535
- std_atomic_mass                  1     18994 4613984 85539
- range_atomic_radius              1     19956 4614947 85542
- wtd_range_FusionHeat             1     21159 4616150 85546
- wtd_mean_ElectronAffinity        1     21260 4616251 85546
- std_Density                      1     21731 4616721 85548
- wtd_entropy_fie                  1     21986 4616977 85549
- wtd_mean_FusionHeat              1     22653 4617644 85551
- mean_atomic_mass                 1     22840 4617831 85551
- range_fie                        1     23456 4618447 85553
- wtd_entropy_ElectronAffinity     1     26790 4621781 85564
- mean_atomic_radius               1     29556 4624547 85573
- wtd_gmean_ElectronAffinity       1     31844 4626835 85580
- wtd_entropy_Valence              1     32211 4627202 85582
- wtd_gmean_ThermalConductivity    1     35445 4630436 85592
- range_atomic_mass                1     37609 4632600 85599
- wtd_entropy_FusionHeat           1     38993 4633984 85603
- wtd_std_ElectronAffinity         1     40398 4635389 85608
- wtd_range_ThermalConductivity    1     41901 4636892 85613
- wtd_std_Valence                  1     43917 4638907 85619
- mean_Density                     1     45450 4640441 85624
```

```
- wtd_gmean_atomic_radius          1     62040 4657031 85677
- wtd_mean_atomic_radius           1     73664 4668654 85714
- wtd_mean_ThermalConductivity     1     78925 4673916 85731
- std_ElectronAffinity             1     99835 4694826 85797
- range_ElectronAffinity           1    103817 4698808 85810

Step:  AIC=85478.12
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + wtd_std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + mean_ElectronAffinity +
    wtd_mean_ElectronAffinity + gmean_ElectronAffinity +
wtd_gmean_ElectronAffinity +
    entropy_ElectronAffinity + wtd_entropy_ElectronAffinity +
    range_ElectronAffinity + wtd_range_ElectronAffinity + std_ElectronAffinity +
    wtd_std_ElectronAffinity + mean_FusionHeat + wtd_mean_FusionHeat +
    gmean_FusionHeat + wtd_gmean_FusionHeat + entropy_FusionHeat +
    wtd_entropy_FusionHeat + range_FusionHeat + wtd_range_FusionHeat +
    std_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    mean_Valence + wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence +
    entropy_Valence + wtd_entropy_Valence + range_Valence + wtd_range_Valence +
    std_Valence + wtd_std_Valence

                                  Df Sum of Sq     RSS   AIC
- wtd_std_fie                      1       139 4595301 85477
- wtd_range_Valence                1       480 4595642 85478
- mean_ElectronAffinity            1       584 4595745 85478
<none>                                       4595161 85478
- std_FusionHeat                   1       656 4595817 85478
- wtd_std_atomic_mass              1       719 4595881 85478
- mean_ThermalConductivity         1       866 4596027 85479
- wtd_entropy_atomic_mass          1       895 4596057 85479
- wtd_entropy_ThermalConductivity  1       943 4596104 85479
- entropy_ElectronAffinity         1      1032 4596193 85479
- wtd_range_atomic_mass            1      1036 4596197 85479
- std_Valence                      1      1364 4596525 85481
- mean_Valence                     1      1880 4597041 85482
```

```
- gmean_fie                        1      2197 4597359 85483
- wtd_mean_fie                     1      2211 4597372 85483
- mean_fie                         1      2211 4597373 85483
- wtd_std_atomic_radius            1      2322 4597484 85484
- gmean_ElectronAffinity           1      2603 4597764 85485
- wtd_gmean_fie                    1      2807 4597968 85485
- gmean_Density                    1      2849 4598010 85485
- gmean_Valence                    1      3152 4598313 85486
- gmean_ThermalConductivity        1      3454 4598615 85487
- wtd_mean_Valence                 1      3593 4598754 85488
- number_of_elements               1      3856 4599017 85489
- wtd_std_FusionHeat               1      3973 4599134 85489
- wtd_std_Density                  1      4144 4599306 85490
- entropy_atomic_radius            1      4919 4600080 85492
- wtd_gmean_Valence                1      5194 4600355 85493
- entropy_Density                  1      5350 4600512 85493
- entropy_ThermalConductivity      1      6041 4601203 85496
- gmean_atomic_mass                1      6616 4601778 85498
- range_FusionHeat                 1      7004 4602165 85499
- wtd_gmean_atomic_mass            1      7583 4602745 85501
- wtd_range_atomic_radius          1      8290 4603451 85503
- entropy_fie                      1      9099 4604261 85506
- entropy_Valence                  1      9247 4604409 85506
- wtd_range_fie                    1      9549 4604710 85507
- entropy_FusionHeat               1      9673 4604835 85507
- std_atomic_radius                1     10073 4605235 85509
- range_ThermalConductivity        1     11402 4606564 85513
- wtd_entropy_atomic_radius        1     11736 4606897 85514
- std_ThermalConductivity          1     12313 4607474 85516
- wtd_range_ElectronAffinity       1     12988 4608150 85518
- range_Valence                    1     13197 4608359 85519
- range_Density                    1     14294 4609456 85522
- wtd_gmean_Density                1     14669 4609830 85524
- gmean_FusionHeat                 1     15132 4610294 85525
- wtd_entropy_Density              1     15173 4610334 85525
- entropy_atomic_mass              1     16074 4611235 85528
- wtd_mean_atomic_mass             1     16418 4611580 85529
- wtd_gmean_FusionHeat             1     16512 4611673 85530
- mean_FusionHeat                  1     16954 4612116 85531
- std_fie                          1     17808 4612970 85534
- std_atomic_mass                  1     19084 4614246 85538
- range_atomic_radius              1     20171 4615332 85541
- wtd_range_FusionHeat             1     21330 4616492 85545
- wtd_mean_ElectronAffinity        1     21466 4616628 85545
- wtd_entropy_fie                  1     21884 4617045 85547
- std_Density                      1     22313 4617474 85548
- wtd_mean_FusionHeat              1     22490 4617651 85549
- mean_atomic_mass                 1     22869 4618030 85550
```

```
- range_fie                          1     23444 4618606 85552
- wtd_entropy_ElectronAffinity      1     27036 4622198 85563
- mean_atomic_radius                1     29386 4624547 85571
- wtd_gmean_ElectronAffinity        1     32591 4627752 85581
- wtd_entropy_Valence               1     32958 4628119 85582
- range_atomic_mass                 1     37515 4632676 85597
- wtd_entropy_FusionHeat            1     38866 4634027 85601
- wtd_std_ElectronAffinity          1     40589 4635750 85607
- wtd_range_ThermalConductivity     1     41815 4636976 85611
- wtd_std_Valence                   1     44934 4640095 85621
- mean_Density                      1     45510 4640672 85623
- wtd_gmean_atomic_radius           1     61898 4657060 85675
- wtd_mean_atomic_radius            1     73501 4668663 85712
- wtd_gmean_ThermalConductivity     1     78375 4673537 85728
- std_ElectronAffinity              1     99808 4694969 85796
- range_ElectronAffinity            1    103706 4698868 85808
- wtd_mean_ThermalConductivity      1    132127 4727288 85898

Step:  AIC=85476.57
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + mean_ElectronAffinity +
    wtd_mean_ElectronAffinity + gmean_ElectronAffinity +
wtd_gmean_ElectronAffinity +
    entropy_ElectronAffinity + wtd_entropy_ElectronAffinity +
    range_ElectronAffinity + wtd_range_ElectronAffinity + std_ElectronAffinity +
    wtd_std_ElectronAffinity + mean_FusionHeat + wtd_mean_FusionHeat +
    gmean_FusionHeat + wtd_gmean_FusionHeat + entropy_FusionHeat +
    wtd_entropy_FusionHeat + range_FusionHeat + wtd_range_FusionHeat +
    std_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    mean_Valence + wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence +
    entropy_Valence + wtd_entropy_Valence + range_Valence + wtd_range_Valence +
    std_Valence + wtd_std_Valence

                                Df Sum of Sq     RSS   AIC
- wtd_range_Valence              1       474 4595775 85476
```

```
- mean_ElectronAffinity            1       601 4595902 85477
<none>                                       4595301 85477
- std_FusionHeat                   1       635 4595936 85477
- wtd_std_atomic_mass              1       710 4596011 85477
- mean_ThermalConductivity         1       810 4596111 85477
- wtd_entropy_atomic_mass          1       893 4596193 85477
- wtd_entropy_ThermalConductivity  1       948 4596248 85478
- entropy_ElectronAffinity         1      1039 4596340 85478
- wtd_range_atomic_mass            1      1068 4596369 85478
- std_Valence                      1      1389 4596689 85479
- mean_Valence                     1      1812 4597113 85480
- wtd_std_atomic_radius            1      2621 4597922 85483
- gmean_ElectronAffinity           1      2661 4597961 85483
- gmean_Density                    1      2748 4598049 85483
- gmean_Valence                    1      3077 4598378 85485
- wtd_mean_Valence                 1      3506 4598807 85486
- gmean_ThermalConductivity        1      3608 4598909 85486
- wtd_std_FusionHeat               1      3836 4599137 85487
- number_of_elements               1      4044 4599344 85488
- wtd_std_Density                  1      4051 4599352 85488
- wtd_gmean_Valence                1      5109 4600410 85491
- entropy_Density                  1      5211 4600512 85491
- entropy_atomic_radius            1      5437 4600738 85492
- entropy_ThermalConductivity      1      5941 4601242 85494
- gmean_fie                        1      5945 4601246 85494
- mean_fie                         1      5986 4601287 85494
- gmean_atomic_mass                1      6676 4601977 85496
- range_FusionHeat                 1      6904 4602204 85497
- wtd_gmean_atomic_mass            1      7542 4602842 85499
- wtd_range_atomic_radius          1      8463 4603764 85502
- entropy_FusionHeat               1      9535 4604836 85505
- wtd_range_fie                    1      9594 4604895 85506
- entropy_Valence                  1      9594 4604895 85506
- std_atomic_radius                1      9944 4605245 85507
- entropy_fie                      1      9946 4605247 85507
- range_ThermalConductivity        1     11561 4606862 85512
- wtd_entropy_atomic_radius        1     11830 4607131 85513
- std_ThermalConductivity          1     12374 4607675 85515
- wtd_range_ElectronAffinity       1     13024 4608325 85517
- range_Valence                    1     13131 4608432 85517
- wtd_mean_fie                     1     13955 4609256 85520
- range_Density                    1     14546 4609847 85522
- wtd_entropy_Density              1     15033 4610334 85523
- gmean_FusionHeat                 1     15066 4610367 85523
- entropy_atomic_mass              1     15961 4611262 85526
- wtd_gmean_fie                    1     16213 4611514 85527
- wtd_gmean_Density                1     16363 4611663 85527
- wtd_gmean_FusionHeat             1     16417 4611718 85528
```

```
- wtd_mean_atomic_mass             1     16471 4611772 85528
- mean_FusionHeat                  1     16925 4612226 85529
- std_atomic_mass                  1     19094 4614395 85536
- range_atomic_radius              1     20393 4615694 85540
- wtd_range_FusionHeat             1     21352 4616653 85544
- wtd_mean_ElectronAffinity        1     21456 4616757 85544
- wtd_entropy_fie                  1     21792 4617093 85545
- std_Density                      1     22280 4617581 85547
- wtd_mean_FusionHeat              1     22401 4617702 85547
- mean_atomic_mass                 1     23134 4618435 85549
- range_fie                        1     23326 4618627 85550
- wtd_entropy_ElectronAffinity     1     27512 4622813 85563
- mean_atomic_radius               1     29985 4625286 85571
- wtd_gmean_ElectronAffinity       1     32557 4627857 85580
- wtd_entropy_Valence              1     33460 4628760 85583
- std_fie                          1     36806 4632107 85593
- range_atomic_mass                1     37483 4632784 85595
- wtd_entropy_FusionHeat           1     38747 4634048 85600
- wtd_range_ThermalConductivity    1     41806 4637107 85609
- wtd_std_ElectronAffinity         1     42031 4637331 85610
- wtd_std_Valence                  1     45027 4640328 85620
- mean_Density                     1     45551 4640852 85621
- wtd_gmean_atomic_radius          1     65522 4660823 85685
- wtd_mean_atomic_radius           1     77313 4672614 85723
- wtd_gmean_ThermalConductivity    1     78960 4674261 85728
- std_ElectronAffinity             1    100096 4695397 85795
- range_ElectronAffinity           1    103932 4699233 85807
- wtd_mean_ThermalConductivity     1    133683 4728984 85901

Step:  AIC=85476.1
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + mean_ElectronAffinity +
    wtd_mean_ElectronAffinity + gmean_ElectronAffinity +
wtd_gmean_ElectronAffinity +
    entropy_ElectronAffinity + wtd_entropy_ElectronAffinity +
    range_ElectronAffinity + wtd_range_ElectronAffinity + std_ElectronAffinity +
    wtd_std_ElectronAffinity + mean_FusionHeat + wtd_mean_FusionHeat +
    gmean_FusionHeat + wtd_gmean_FusionHeat + entropy_FusionHeat +
    wtd_entropy_FusionHeat + range_FusionHeat + wtd_range_FusionHeat +
```

```
    std_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    mean_Valence + wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence +
    entropy_Valence + wtd_entropy_Valence + range_Valence + std_Valence +
    wtd_std_Valence

                                 Df Sum of Sq     RSS   AIC
- std_FusionHeat                  1       507 4596282 85476
- mean_ElectronAffinity           1       516 4596291 85476
<none>                                       4595775 85476
- wtd_std_atomic_mass             1       739 4596514 85476
- wtd_entropy_atomic_mass         1       767 4596542 85477
- mean_ThermalConductivity        1       812 4596587 85477
- wtd_range_atomic_mass           1       873 4596648 85477
- wtd_entropy_ThermalConductivity 1       941 4596716 85477
- entropy_ElectronAffinity        1      1060 4596835 85478
- std_Valence                     1      1193 4596967 85478
- mean_Valence                    1      1643 4597417 85479
- gmean_ElectronAffinity          1      2427 4598202 85482
- wtd_std_atomic_radius           1      2495 4598270 85482
- gmean_Density                   1      2799 4598574 85483
- gmean_Valence                   1      2909 4598683 85484
- wtd_mean_Valence                1      3175 4598950 85484
- gmean_ThermalConductivity       1      3650 4599425 85486
- wtd_std_FusionHeat              1      3681 4599456 85486
- wtd_std_Density                 1      3921 4599696 85487
- number_of_elements              1      4375 4600149 85488
- wtd_gmean_Valence               1      4806 4600581 85490
- entropy_Density                 1      5208 4600983 85491
- entropy_atomic_radius           1      5364 4601139 85491
- entropy_ThermalConductivity     1      6166 4601940 85494
- gmean_fie                       1      6331 4602106 85495
- mean_fie                        1      6339 4602113 85495
- gmean_atomic_mass               1      6894 4602669 85496
- range_FusionHeat                1      7640 4603415 85499
- wtd_gmean_atomic_mass           1      7658 4603433 85499
- entropy_Valence                 1      9226 4605000 85504
- wtd_range_fie                   1      9390 4605164 85504
- entropy_FusionHeat              1      9469 4605244 85505
- entropy_fie                     1      9603 4605378 85505
- std_atomic_radius               1     10053 4605828 85507
- wtd_range_atomic_radius         1     11336 4607111 85511
- wtd_entropy_atomic_radius       1     11380 4607154 85511
- range_ThermalConductivity       1     11597 4607372 85512
- std_ThermalConductivity         1     12527 4608302 85515
```

```
- range_Valence                   1     13086 4608861 85516
- wtd_mean_fie                    1     13705 4609480 85518
- range_Density                   1     14409 4610183 85521
- wtd_range_ElectronAffinity      1     14769 4610544 85522
- wtd_entropy_Density             1     14805 4610579 85522
- gmean_FusionHeat                1     14999 4610774 85523
- entropy_atomic_mass             1     15762 4611537 85525
- wtd_gmean_fie                   1     16052 4611827 85526
- wtd_gmean_FusionHeat            1     16078 4611853 85526
- wtd_gmean_Density               1     16134 4611909 85526
- wtd_mean_atomic_mass            1     16445 4612220 85527
- mean_FusionHeat                 1     16609 4612384 85528
- std_atomic_mass                 1     19154 4614929 85536
- range_atomic_radius             1     20456 4616231 85540
- wtd_range_FusionHeat            1     20974 4616749 85542
- wtd_mean_ElectronAffinity       1     21273 4617048 85543
- wtd_entropy_fie                 1     21696 4617470 85544
- wtd_mean_FusionHeat             1     21927 4617702 85545
- std_Density                     1     21989 4617764 85545
- range_fie                       1     23128 4618902 85549
- mean_atomic_mass                1     23365 4619140 85550
- wtd_entropy_ElectronAffinity    1     28095 4623870 85565
- mean_atomic_radius              1     29654 4625428 85570
- wtd_gmean_ElectronAffinity      1     32104 4627878 85578
- std_fie                         1     36603 4632378 85592
- wtd_entropy_Valence             1     36862 4632637 85593
- range_atomic_mass               1     37538 4633312 85595
- wtd_entropy_FusionHeat          1     38275 4634050 85598
- wtd_std_ElectronAffinity        1     41588 4637363 85608
- wtd_range_ThermalConductivity   1     41814 4637589 85609
- wtd_std_Valence                 1     44656 4640430 85618
- mean_Density                    1     45641 4641415 85621
- wtd_gmean_atomic_radius         1     65073 4660848 85683
- wtd_mean_atomic_radius          1     76855 4672630 85721
- wtd_gmean_ThermalConductivity   1     78522 4674296 85726
- std_ElectronAffinity            1     99887 4695661 85794
- range_ElectronAffinity          1    104303 4700078 85808
- wtd_mean_ThermalConductivity    1    133211 4728986 85899

Step:  AIC=85475.75
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
```

```
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + mean_ElectronAffinity +
    wtd_mean_ElectronAffinity + gmean_ElectronAffinity +
wtd_gmean_ElectronAffinity +
    entropy_ElectronAffinity + wtd_entropy_ElectronAffinity +
    range_ElectronAffinity + wtd_range_ElectronAffinity + std_ElectronAffinity +
    wtd_std_ElectronAffinity + mean_FusionHeat + wtd_mean_FusionHeat +
    gmean_FusionHeat + wtd_gmean_FusionHeat + entropy_FusionHeat +
    wtd_entropy_FusionHeat + range_FusionHeat + wtd_range_FusionHeat +
    wtd_std_FusionHeat + mean_ThermalConductivity + wtd_mean_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    entropy_ThermalConductivity + wtd_entropy_ThermalConductivity +
    range_ThermalConductivity + wtd_range_ThermalConductivity +
    std_ThermalConductivity + mean_Valence + wtd_mean_Valence +
    gmean_Valence + wtd_gmean_Valence + entropy_Valence + wtd_entropy_Valence +
    range_Valence + std_Valence + wtd_std_Valence

                                  Df Sum of Sq     RSS   AIC
- mean_ElectronAffinity            1       501 4596783 85475
<none>                                       4596282 85476
- wtd_std_atomic_mass              1       687 4596969 85476
- wtd_entropy_atomic_mass          1       724 4597006 85476
- mean_ThermalConductivity         1       813 4597095 85476
- wtd_range_atomic_mass            1       862 4597144 85477
- wtd_entropy_ThermalConductivity  1       976 4597258 85477
- entropy_ElectronAffinity         1      1083 4597365 85477
- std_Valence                      1      1092 4597374 85477
- mean_Valence                     1      1591 4597873 85479
- wtd_std_atomic_radius            1      2322 4598604 85481
- gmean_ElectronAffinity           1      2407 4598689 85482
- gmean_Density                    1      2686 4598968 85482
- gmean_Valence                    1      2832 4599114 85483
- wtd_mean_Valence                 1      3213 4599495 85484
- wtd_std_Density                  1      3822 4600104 85486
- gmean_ThermalConductivity        1      3849 4600131 85486
- wtd_std_FusionHeat               1      3911 4600193 85486
- number_of_elements               1      4202 4600484 85487
- wtd_gmean_Valence                1      4847 4601129 85489
- entropy_Density                  1      4908 4601190 85490
- entropy_atomic_radius            1      5143 4601425 85490
- gmean_fie                        1      6146 4602428 85494
- mean_fie                         1      6178 4602460 85494
- entropy_ThermalConductivity      1      6235 4602517 85494
- gmean_atomic_mass                1      6835 4603117 85496
- wtd_gmean_atomic_mass            1      7538 4603820 85498
- entropy_FusionHeat               1      9062 4605344 85503
```

```
- entropy_Valence                  1      9686 4605968 85505
- wtd_range_fie                    1      9733 4606015 85505
- entropy_fie                      1      9778 4606060 85505
- std_atomic_radius                1     10303 4606585 85507
- wtd_range_atomic_radius          1     11025 4607307 85509
- range_ThermalConductivity        1     11740 4608022 85512
- wtd_entropy_atomic_radius        1     11895 4608177 85512
- std_ThermalConductivity          1     12696 4608978 85515
- range_Valence                    1     13628 4609910 85518
- wtd_mean_fie                     1     13661 4609943 85518
- range_Density                    1     14140 4610422 85519
- wtd_entropy_Density              1     14504 4610786 85521
- wtd_range_ElectronAffinity       1     14697 4610979 85521
- entropy_atomic_mass              1     15487 4611769 85524
- wtd_gmean_fie                    1     15967 4612249 85525
- wtd_gmean_Density                1     16188 4612470 85526
- wtd_mean_atomic_mass             1     16259 4612541 85526
- wtd_gmean_FusionHeat             1     17445 4613727 85530
- gmean_FusionHeat                 1     18288 4614570 85533
- std_atomic_mass                  1     19139 4615421 85536
- range_atomic_radius              1     20199 4616481 85539
- wtd_mean_ElectronAffinity        1     21049 4617331 85542
- wtd_entropy_fie                  1     21517 4617799 85543
- std_Density                      1     21541 4617823 85543
- mean_FusionHeat                  1     23025 4619307 85548
- mean_atomic_mass                 1     23083 4619365 85548
- wtd_range_FusionHeat             1     23366 4619648 85549
- range_fie                        1     23640 4619922 85550
- wtd_mean_FusionHeat              1     26456 4622738 85559
- wtd_entropy_ElectronAffinity     1     28029 4624311 85564
- mean_atomic_radius               1     29193 4625475 85568
- range_FusionHeat                 1     29670 4625952 85570
- wtd_gmean_ElectronAffinity       1     31867 4628149 85577
- wtd_entropy_Valence              1     36391 4632673 85591
- std_fie                          1     37095 4633377 85593
- range_atomic_mass                1     38109 4634391 85597
- wtd_entropy_FusionHeat           1     40528 4636810 85604
- wtd_std_ElectronAffinity         1     41473 4637755 85607
- wtd_range_ThermalConductivity    1     42201 4638483 85610
- wtd_std_Valence                  1     44391 4640673 85617
- mean_Density                     1     45157 4641439 85619
- wtd_gmean_atomic_radius          1     64735 4661017 85682
- wtd_mean_atomic_radius           1     76453 4672735 85719
- wtd_gmean_ThermalConductivity    1     78324 4674606 85725
- std_ElectronAffinity             1     99628 4695910 85793
- range_ElectronAffinity           1    104121 4700403 85807
- wtd_mean_ThermalConductivity     1    133758 4730040 85901
```

```
Step:  AIC=85475.37
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + wtd_std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + wtd_mean_ElectronAffinity +
    gmean_ElectronAffinity + wtd_gmean_ElectronAffinity +
entropy_ElectronAffinity +
    wtd_entropy_ElectronAffinity + range_ElectronAffinity +
wtd_range_ElectronAffinity +
    std_ElectronAffinity + wtd_std_ElectronAffinity + mean_FusionHeat +
    wtd_mean_FusionHeat + gmean_FusionHeat + wtd_gmean_FusionHeat +
    entropy_FusionHeat + wtd_entropy_FusionHeat + range_FusionHeat +
    wtd_range_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    mean_Valence + wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence +
    entropy_Valence + wtd_entropy_Valence + range_Valence + std_Valence +
    wtd_std_Valence

                                  Df Sum of Sq     RSS   AIC
- wtd_std_atomic_mass              1       581 4597364 85475
<none>                                       4596783 85475
- wtd_entropy_atomic_mass          1       767 4597550 85476
- wtd_range_atomic_mass            1       903 4597686 85476
- mean_ThermalConductivity         1      1091 4597874 85477
- wtd_entropy_ThermalConductivity  1      1175 4597958 85477
- entropy_ElectronAffinity         1      1182 4597965 85477
- std_Valence                      1      1224 4598007 85477
- mean_Valence                     1      1761 4598544 85479
- wtd_std_atomic_radius            1      2254 4599037 85481
- gmean_Density                    1      2913 4599696 85483
- gmean_Valence                    1      3028 4599811 85483
- wtd_mean_Valence                 1      3564 4600347 85485
- gmean_ThermalConductivity        1      3647 4600430 85485
- wtd_std_Density                  1      3766 4600549 85486
- number_of_elements               1      3912 4600695 85486
- wtd_std_FusionHeat               1      3956 4600739 85486
- gmean_ElectronAffinity           1      4316 4601099 85487
- entropy_atomic_radius            1      4871 4601654 85489
```

```
- entropy_Density                  1      4876 4601659 85489
- wtd_gmean_Valence                1      5262 4602045 85490
- mean_fie                         1      6095 4602878 85493
- gmean_fie                        1      6210 4602993 85493
- entropy_ThermalConductivity      1      6332 4603115 85494
- gmean_atomic_mass                1      6842 4603625 85496
- wtd_gmean_atomic_mass            1      7479 4604262 85498
- wtd_range_fie                    1      9469 4606253 85504
- entropy_fie                      1      9643 4606426 85505
- entropy_FusionHeat               1      9731 4606514 85505
- entropy_Valence                  1     10109 4606892 85506
- std_atomic_radius                1     10493 4607276 85507
- wtd_range_atomic_radius          1     10900 4607684 85509
- range_ThermalConductivity        1     12093 4608876 85512
- wtd_entropy_atomic_radius        1     12175 4608958 85513
- std_ThermalConductivity          1     13229 4610012 85516
- range_Valence                    1     13834 4610617 85518
- range_Density                    1     14063 4610846 85519
- wtd_range_ElectronAffinity       1     14230 4611013 85519
- wtd_entropy_Density              1     14641 4611424 85521
- wtd_mean_fie                     1     14770 4611553 85521
- entropy_atomic_mass              1     15553 4612336 85524
- wtd_gmean_Density                1     15849 4612632 85525
- wtd_mean_atomic_mass             1     16104 4612887 85525
- wtd_gmean_FusionHeat             1     17459 4614242 85530
- wtd_gmean_fie                    1     17559 4614342 85530
- gmean_FusionHeat                 1     18416 4615199 85533
- std_atomic_mass                  1     18752 4615535 85534
- range_atomic_radius              1     19843 4616626 85537
- wtd_entropy_fie                  1     21494 4618277 85543
- std_Density                      1     21503 4618286 85543
- mean_atomic_mass                 1     22945 4619729 85547
- mean_FusionHeat                  1     23353 4620136 85549
- wtd_range_FusionHeat             1     23946 4620729 85551
- range_fie                        1     24923 4621706 85554
- wtd_mean_FusionHeat              1     26636 4623419 85559
- mean_atomic_radius               1     29585 4626368 85569
- wtd_entropy_ElectronAffinity     1     30003 4626786 85570
- range_FusionHeat                 1     30773 4627556 85573
- wtd_mean_ElectronAffinity        1     33993 4630776 85583
- wtd_entropy_Valence              1     36535 4633318 85591
- std_fie                          1     37680 4634463 85595
- range_atomic_mass                1     37788 4634571 85595
- wtd_entropy_FusionHeat           1     41730 4638513 85608
- wtd_range_ThermalConductivity    1     41991 4638774 85609
- wtd_gmean_ElectronAffinity       1     45225 4642008 85619
- mean_Density                     1     45346 4642129 85619
- wtd_std_Valence                  1     47198 4643981 85625
```

```
- wtd_std_ElectronAffinity         1     50209 4646992 85635
- wtd_gmean_atomic_radius          1     66448 4663231 85687
- wtd_mean_atomic_radius           1     78267 4675050 85725
- wtd_gmean_ThermalConductivity    1     78489 4675272 85725
- range_ElectronAffinity           1    105624 4702407 85812
- std_ElectronAffinity             1    112767 4709550 85834
- wtd_mean_ThermalConductivity     1    135498 4732281 85906

Step:  AIC=85475.25
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    wtd_entropy_atomic_mass + range_atomic_mass + wtd_range_atomic_mass +
    std_atomic_mass + mean_fie + wtd_mean_fie + gmean_fie + wtd_gmean_fie +
    entropy_fie + wtd_entropy_fie + range_fie + wtd_range_fie +
    std_fie + mean_atomic_radius + wtd_mean_atomic_radius +
wtd_gmean_atomic_radius +
    entropy_atomic_radius + wtd_entropy_atomic_radius + range_atomic_radius +
    wtd_range_atomic_radius + std_atomic_radius + wtd_std_atomic_radius +
    mean_Density + gmean_Density + wtd_gmean_Density + entropy_Density +
    wtd_entropy_Density + range_Density + std_Density + wtd_std_Density +
    wtd_mean_ElectronAffinity + gmean_ElectronAffinity +
wtd_gmean_ElectronAffinity +
    entropy_ElectronAffinity + wtd_entropy_ElectronAffinity +
    range_ElectronAffinity + wtd_range_ElectronAffinity + std_ElectronAffinity +
    wtd_std_ElectronAffinity + mean_FusionHeat + wtd_mean_FusionHeat +
    gmean_FusionHeat + wtd_gmean_FusionHeat + entropy_FusionHeat +
    wtd_entropy_FusionHeat + range_FusionHeat + wtd_range_FusionHeat +
    wtd_std_FusionHeat + mean_ThermalConductivity + wtd_mean_ThermalConductivity
+
    gmean_ThermalConductivity + wtd_gmean_ThermalConductivity +
    entropy_ThermalConductivity + wtd_entropy_ThermalConductivity +
    range_ThermalConductivity + wtd_range_ThermalConductivity +
    std_ThermalConductivity + mean_Valence + wtd_mean_Valence +
    gmean_Valence + wtd_gmean_Valence + entropy_Valence + wtd_entropy_Valence +
    range_Valence + std_Valence + wtd_std_Valence

                                  Df Sum of Sq     RSS   AIC
- wtd_entropy_atomic_mass          1       585 4597950 85475
<none>                                       4597364 85475
- wtd_range_atomic_mass            1       767 4598131 85476
- std_Valence                      1       964 4598328 85476
- wtd_entropy_ThermalConductivity  1      1069 4598434 85477
- mean_ThermalConductivity         1      1168 4598532 85477
- entropy_ElectronAffinity         1      1193 4598557 85477
- mean_Valence                     1      1394 4598758 85478
- wtd_std_atomic_radius            1      2275 4599639 85481
- gmean_Valence                    1      2596 4599960 85482
- gmean_Density                    1      2820 4600184 85482
```

```
- wtd_mean_Valence                1      3031 4600396 85483
- wtd_std_Density                 1      3186 4600551 85484
- gmean_ThermalConductivity       1      3466 4600830 85484
- wtd_std_FusionHeat              1      3725 4601089 85485
- number_of_elements              1      3986 4601350 85486
- gmean_ElectronAffinity          1      4019 4601383 85486
- entropy_Density                 1      4456 4601820 85488
- entropy_atomic_radius           1      4625 4601989 85488
- wtd_gmean_Valence               1      4694 4602059 85488
- mean_fie                        1      6122 4603486 85493
- gmean_fie                       1      6252 4603616 85493
- entropy_ThermalConductivity     1      6357 4603721 85494
- gmean_atomic_mass               1      6814 4604178 85495
- entropy_fie                     1      9519 4606883 85504
- entropy_FusionHeat              1      9542 4606907 85504
- wtd_gmean_atomic_mass           1      9797 4607161 85505
- entropy_Valence                 1     10287 4607652 85507
- std_atomic_radius               1     10504 4607868 85507
- wtd_range_fie                   1     10717 4608081 85508
- wtd_range_atomic_radius         1     11711 4609075 85511
- range_ThermalConductivity       1     12059 4609424 85512
- wtd_entropy_atomic_radius       1     12336 4609700 85513
- std_ThermalConductivity         1     13291 4610656 85516
- wtd_entropy_Density             1     14147 4611511 85519
- range_Valence                   1     14364 4611728 85520
- wtd_mean_fie                    1     14385 4611749 85520
- entropy_atomic_mass             1     14972 4612337 85522
- wtd_range_ElectronAffinity      1     15012 4612376 85522
- range_Density                   1     15068 4612432 85522
- wtd_gmean_Density               1     16346 4613710 85526
- wtd_gmean_fie                   1     17127 4614492 85529
- wtd_gmean_FusionHeat            1     17129 4614493 85529
- gmean_FusionHeat                1     18257 4615621 85532
- range_atomic_radius             1     20425 4617789 85539
- std_Density                     1     20974 4618339 85541
- wtd_entropy_fie                 1     22840 4620205 85547
- mean_FusionHeat                 1     23424 4620788 85549
- wtd_mean_atomic_mass            1     23690 4621054 85550
- wtd_range_FusionHeat            1     24407 4621771 85552
- range_fie                       1     25191 4622555 85555
- wtd_mean_FusionHeat             1     26413 4623777 85559
- mean_atomic_mass                1     27155 4624520 85561
- std_atomic_mass                 1     27604 4624968 85562
- wtd_entropy_ElectronAffinity    1     29709 4627073 85569
- mean_atomic_radius              1     29888 4627252 85570
- range_FusionHeat                1     30610 4627974 85572
- wtd_mean_ElectronAffinity       1     34671 4632035 85585
- range_atomic_mass               1     37504 4634869 85594
```

```
- std_fie                           1     38117 4635481 85596
- wtd_entropy_Valence               1     38269 4635633 85597
- wtd_entropy_FusionHeat            1     41219 4638583 85606
- wtd_range_ThermalConductivity     1     41973 4639338 85609
- wtd_gmean_ElectronAffinity        1     45029 4642393 85618
- mean_Density                      1     45333 4642697 85619
- wtd_std_Valence                   1     47441 4644806 85626
- wtd_std_ElectronAffinity          1     49646 4647011 85633
- wtd_gmean_atomic_radius           1     65880 4663245 85685
- wtd_mean_atomic_radius            1     77691 4675055 85723
- wtd_gmean_ThermalConductivity     1     78546 4675910 85725
- range_ElectronAffinity            1    107296 4704660 85817
- std_ElectronAffinity              1    112978 4710342 85835
- wtd_mean_ThermalConductivity      1    135404 4732768 85905

Step:  AIC=85475.15
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    range_atomic_mass + wtd_range_atomic_mass + std_atomic_mass +
    mean_fie + wtd_mean_fie + gmean_fie + wtd_gmean_fie + entropy_fie +
    wtd_entropy_fie + range_fie + wtd_range_fie + std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + wtd_mean_ElectronAffinity +
    gmean_ElectronAffinity + wtd_gmean_ElectronAffinity +
entropy_ElectronAffinity +
    wtd_entropy_ElectronAffinity + range_ElectronAffinity +
wtd_range_ElectronAffinity +
    std_ElectronAffinity + wtd_std_ElectronAffinity + mean_FusionHeat +
    wtd_mean_FusionHeat + gmean_FusionHeat + wtd_gmean_FusionHeat +
    entropy_FusionHeat + wtd_entropy_FusionHeat + range_FusionHeat +
    wtd_range_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    mean_Valence + wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence +
    entropy_Valence + wtd_entropy_Valence + range_Valence + std_Valence +
    wtd_std_Valence

                                  Df Sum of Sq     RSS   AIC
- wtd_range_atomic_mass            1       438 4598388 85475
<none>                                       4597950 85475
- wtd_entropy_ThermalConductivity  1       895 4598845 85476
- entropy_ElectronAffinity         1      1060 4599010 85477
- std_Valence                      1      1127 4599077 85477
```

```
- mean_ThermalConductivity         1      1290 4599240 85477
- mean_Valence                     1      1361 4599311 85478
- wtd_std_atomic_radius            1      2306 4600256 85481
- gmean_Valence                    1      2551 4600500 85481
- gmean_Density                    1      2680 4600630 85482
- wtd_std_Density                  1      2808 4600758 85482
- wtd_mean_Valence                 1      3112 4601061 85483
- gmean_ThermalConductivity        1      3226 4601175 85484
- wtd_std_FusionHeat               1      3437 4601386 85484
- number_of_elements               1      4139 4602088 85487
- entropy_Density                  1      4141 4602090 85487
- entropy_atomic_radius            1      4293 4602243 85487
- gmean_ElectronAffinity           1      4314 4602263 85487
- wtd_gmean_Valence                1      4802 4602752 85489
- mean_fie                         1      6003 4603953 85493
- gmean_fie                        1      6140 4604090 85493
- entropy_ThermalConductivity      1      6970 4604920 85496
- gmean_atomic_mass                1      8643 4606593 85501
- entropy_fie                      1      9579 4607529 85504
- entropy_FusionHeat               1      9681 4607631 85504
- std_atomic_radius                1     10586 4608536 85507
- wtd_range_fie                    1     10792 4608741 85508
- entropy_Valence                  1     10897 4608847 85508
- wtd_range_atomic_radius          1     11127 4609077 85509
- range_ThermalConductivity        1     11920 4609870 85512
- std_ThermalConductivity          1     13205 4611155 85516
- range_Valence                    1     14110 4612060 85519
- wtd_entropy_Density              1     14150 4612100 85519
- wtd_mean_fie                     1     14498 4612448 85520
- range_Density                    1     14839 4612789 85521
- entropy_atomic_mass              1     14981 4612930 85522
- wtd_range_ElectronAffinity       1     15397 4613347 85523
- wtd_gmean_atomic_mass            1     16148 4614097 85525
- wtd_gmean_Density                1     17243 4615193 85529
- wtd_gmean_FusionHeat             1     17294 4615244 85529
- wtd_gmean_fie                    1     17314 4615263 85529
- gmean_FusionHeat                 1     18824 4616773 85534
- range_atomic_radius              1     20250 4618199 85539
- std_Density                      1     20454 4618403 85539
- wtd_entropy_fie                  1     22436 4620386 85546
- mean_FusionHeat                  1     23819 4621768 85550
- wtd_range_FusionHeat             1     24495 4622445 85552
- range_fie                        1     25563 4623513 85556
- wtd_mean_FusionHeat              1     26437 4624387 85558
- wtd_entropy_atomic_radius        1     26484 4624434 85559
- std_atomic_mass                  1     27027 4624977 85560
- wtd_entropy_ElectronAffinity     1     29298 4627248 85568
- range_FusionHeat                 1     30480 4628430 85571
```

```
- mean_atomic_radius               1     31391 4629340 85574
- wtd_mean_ElectronAffinity        1     35085 4633035 85586
- mean_atomic_mass                 1     36064 4634014 85589
- range_atomic_mass                1     36972 4634922 85592
- wtd_entropy_Valence              1     38362 4636311 85597
- std_fie                          1     38827 4636777 85598
- wtd_mean_atomic_mass             1     39532 4637481 85601
- wtd_entropy_FusionHeat           1     40711 4638661 85604
- wtd_range_ThermalConductivity    1     41514 4639464 85607
- mean_Density                     1     45918 4643867 85621
- wtd_gmean_ElectronAffinity       1     46074 4644023 85622
- wtd_std_Valence                  1     49187 4647136 85632
- wtd_std_ElectronAffinity         1     49192 4647141 85632
- wtd_gmean_atomic_radius          1     67937 4665887 85691
- wtd_gmean_ThermalConductivity    1     79970 4677920 85730
- wtd_mean_atomic_radius           1     80180 4678129 85730
- range_ElectronAffinity           1    106719 4704669 85815
- std_ElectronAffinity             1    112394 4710344 85833
- wtd_mean_ThermalConductivity     1    136416 4734366 85908

Step:  AIC=85474.56
critical_temp ~ number_of_elements + mean_atomic_mass + wtd_mean_atomic_mass +
    gmean_atomic_mass + wtd_gmean_atomic_mass + entropy_atomic_mass +
    range_atomic_mass + std_atomic_mass + mean_fie + wtd_mean_fie +
    gmean_fie + wtd_gmean_fie + entropy_fie + wtd_entropy_fie +
    range_fie + wtd_range_fie + std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + wtd_mean_ElectronAffinity +
    gmean_ElectronAffinity + wtd_gmean_ElectronAffinity +
entropy_ElectronAffinity +
    wtd_entropy_ElectronAffinity + range_ElectronAffinity +
wtd_range_ElectronAffinity +
    std_ElectronAffinity + wtd_std_ElectronAffinity + mean_FusionHeat +
    wtd_mean_FusionHeat + gmean_FusionHeat + wtd_gmean_FusionHeat +
    entropy_FusionHeat + wtd_entropy_FusionHeat + range_FusionHeat +
    wtd_range_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    mean_Valence + wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence +
    entropy_Valence + wtd_entropy_Valence + range_Valence + std_Valence +
    wtd_std_Valence

                                Df Sum of Sq     RSS   AIC
```

```
<none>                                    4598388 85475
- wtd_entropy_ThermalConductivity  1       902 4599290 85475
- entropy_ElectronAffinity         1       993 4599380 85476
- std_Valence                      1      1257 4599644 85477
- mean_ThermalConductivity         1      1336 4599724 85477
- mean_Valence                     1      1529 4599917 85478
- wtd_std_atomic_radius            1      2120 4600507 85479
- gmean_Density                    1      2652 4601039 85481
- gmean_Valence                    1      2784 4601172 85482
- wtd_std_Density                  1      3198 4601585 85483
- gmean_ThermalConductivity        1      3385 4601772 85484
- wtd_mean_Valence                 1      3454 4601842 85484
- wtd_std_FusionHeat               1      3527 4601915 85484
- number_of_elements               1      4092 4602479 85486
- entropy_atomic_radius            1      4170 4602558 85486
- entropy_Density                  1      4490 4602878 85487
- gmean_ElectronAffinity           1      4797 4603185 85488
- wtd_gmean_Valence                1      5255 4603642 85490
- mean_fie                         1      6053 4604440 85492
- gmean_fie                        1      6153 4604541 85492
- entropy_ThermalConductivity      1      6947 4605335 85495
- gmean_atomic_mass                1      9031 4607418 85502
- entropy_fie                      1      9505 4607893 85503
- entropy_FusionHeat               1      9818 4608205 85504
- entropy_Valence                  1     10892 4609280 85508
- std_atomic_radius                1     10965 4609353 85508
- wtd_range_fie                    1     11258 4609646 85509
- range_ThermalConductivity        1     11956 4610343 85511
- wtd_range_atomic_radius          1     12183 4610570 85512
- std_ThermalConductivity          1     13242 4611630 85515
- range_Valence                    1     13991 4612378 85518
- wtd_mean_fie                     1     14518 4612906 85519
- entropy_atomic_mass              1     14727 4613115 85520
- range_Density                    1     14992 4613379 85521
- wtd_range_ElectronAffinity       1     15014 4613402 85521
- wtd_entropy_Density              1     15621 4614009 85523
- wtd_gmean_atomic_mass            1     15785 4614173 85524
- wtd_gmean_FusionHeat             1     17052 4615439 85528
- wtd_gmean_Density                1     17144 4615532 85528
- wtd_gmean_fie                    1     17237 4615625 85528
- gmean_FusionHeat                 1     18602 4616989 85533
- range_atomic_radius              1     20091 4618479 85537
- std_Density                      1     21201 4619588 85541
- wtd_entropy_fie                  1     22338 4620726 85545
- mean_FusionHeat                  1     23706 4622094 85549
- wtd_range_FusionHeat             1     24156 4622543 85551
- range_fie                        1     25402 4623789 85555
- wtd_mean_FusionHeat              1     26136 4624524 85557
```

```
- std_atomic_mass                  1     26656 4625044 85559
- wtd_entropy_atomic_radius        1     26896 4625283 85559
- wtd_entropy_ElectronAffinity     1     28913 4627301 85566
- range_FusionHeat                 1     30835 4629222 85572
- mean_atomic_radius               1     31532 4629919 85574
- wtd_mean_ElectronAffinity        1     34816 4633204 85585
- mean_atomic_mass                 1     35641 4634028 85587
- range_atomic_mass                1     36806 4635193 85591
- wtd_entropy_Valence              1     38073 4636461 85595
- std_fie                          1     38724 4637111 85597
- wtd_entropy_FusionHeat           1     40785 4639173 85604
- wtd_mean_atomic_mass             1     43548 4641936 85613
- wtd_range_ThermalConductivity    1     43891 4642279 85614
- mean_Density                     1     45831 4644219 85620
- wtd_gmean_ElectronAffinity       1     47104 4645491 85624
- wtd_std_ElectronAffinity         1     50339 4648727 85635
- wtd_std_Valence                  1     50486 4648874 85635
- wtd_gmean_atomic_radius          1     67499 4665887 85689
- wtd_gmean_ThermalConductivity    1     80013 4678401 85729
- wtd_mean_atomic_radius           1     80150 4678538 85730
- range_ElectronAffinity           1    106474 4704861 85813
- std_ElectronAffinity             1    112327 4710714 85832
- wtd_mean_ThermalConductivity     1    141946 4740334 85925

Call:
lm(formula = critical_temp ~ number_of_elements + mean_atomic_mass +
    wtd_mean_atomic_mass + gmean_atomic_mass + wtd_gmean_atomic_mass +
    entropy_atomic_mass + range_atomic_mass + std_atomic_mass +
    mean_fie + wtd_mean_fie + gmean_fie + wtd_gmean_fie + entropy_fie +
    wtd_entropy_fie + range_fie + wtd_range_fie + std_fie + mean_atomic_radius +
    wtd_mean_atomic_radius + wtd_gmean_atomic_radius + entropy_atomic_radius +
    wtd_entropy_atomic_radius + range_atomic_radius + wtd_range_atomic_radius +
    std_atomic_radius + wtd_std_atomic_radius + mean_Density +
    gmean_Density + wtd_gmean_Density + entropy_Density + wtd_entropy_Density +
    range_Density + std_Density + wtd_std_Density + wtd_mean_ElectronAffinity +
    gmean_ElectronAffinity + wtd_gmean_ElectronAffinity + entropy_ElectronAffinity +
    wtd_entropy_ElectronAffinity + range_ElectronAffinity + wtd_range_ElectronAffinity +
    std_ElectronAffinity + wtd_std_ElectronAffinity + mean_FusionHeat +
    wtd_mean_FusionHeat + gmean_FusionHeat + wtd_gmean_FusionHeat +
    entropy_FusionHeat + wtd_entropy_FusionHeat + range_FusionHeat +
    wtd_range_FusionHeat + wtd_std_FusionHeat + mean_ThermalConductivity +
    wtd_mean_ThermalConductivity + gmean_ThermalConductivity +
    wtd_gmean_ThermalConductivity + entropy_ThermalConductivity +
    wtd_entropy_ThermalConductivity + range_ThermalConductivity +
    wtd_range_ThermalConductivity + std_ThermalConductivity +
    mean_Valence + wtd_mean_Valence + gmean_Valence + wtd_gmean_Valence +
    entropy_Valence + wtd_entropy_Valence + range_Valence + std_Valence +
    wtd_std_Valence, data = train)
```

```
Residuals:
    Min      1Q  Median      3Q     Max
-84.670  -9.424   0.544  10.953 169.681

Coefficients:
                                Estimate Std. Error t value Pr(>|t|)
(Intercept)                   -2.255e+01  5.810e+00  -3.881 0.000104 ***
number_of_elements            -3.138e+00  8.643e-01  -3.631 0.000284 ***
mean_atomic_mass               7.706e-01  7.192e-02  10.715  < 2e-16 ***
wtd_mean_atomic_mass          -7.381e-01  6.231e-02 -11.844  < 2e-16 ***
gmean_atomic_mass             -4.124e-01  7.647e-02  -5.394 7.01e-08 ***
wtd_gmean_atomic_mass          4.761e-01  6.676e-02   7.131 1.04e-12 ***
entropy_atomic_mass           -3.370e+01  4.893e+00  -6.888 5.89e-12 ***
range_atomic_mass              2.137e-01  1.963e-02  10.889  < 2e-16 ***
std_atomic_mass               -4.915e-01  5.304e-02  -9.267  < 2e-16 ***
mean_fie                       2.297e-01  5.201e-02   4.416 1.01e-05 ***
wtd_mean_fie                  -2.897e-01  4.236e-02  -6.839 8.30e-12 ***
gmean_fie                     -2.281e-01  5.124e-02  -4.452 8.56e-06 ***
wtd_gmean_fie                  3.169e-01  4.253e-02   7.452 9.72e-14 ***
entropy_fie                   -1.268e+02  2.292e+01  -5.533 3.19e-08 ***
wtd_entropy_fie                4.458e+01  5.255e+00   8.483  < 2e-16 ***
range_fie                      6.943e-02  7.676e-03   9.046  < 2e-16 ***
wtd_range_fie                  2.327e-02  3.865e-03   6.022 1.76e-09 ***
std_fie                       -2.183e-01  1.954e-02 -11.169  < 2e-16 ***
mean_atomic_radius            -3.348e-01  3.322e-02 -10.078  < 2e-16 ***
wtd_mean_atomic_radius         2.936e+00  1.827e-01  16.068  < 2e-16 ***
wtd_gmean_atomic_radius       -2.541e+00  1.723e-01 -14.746  < 2e-16 ***
entropy_atomic_radius          7.396e+01  2.018e+01   3.665 0.000248 ***
wtd_entropy_atomic_radius      4.364e+01  4.688e+00   9.308  < 2e-16 ***
range_atomic_radius            2.096e-01  2.605e-02   8.045 9.29e-16 ***
wtd_range_atomic_radius       -9.162e-02  1.463e-02  -6.265 3.84e-10 ***
std_atomic_radius             -5.035e-01  8.471e-02  -5.943 2.86e-09 ***
wtd_std_atomic_radius         -1.922e-01  7.354e-02  -2.613 0.008984 **
mean_Density                  -5.046e-03  4.153e-04 -12.151  < 2e-16 ***
gmean_Density                  1.231e-03  4.214e-04   2.923 0.003475 **
wtd_gmean_Density              2.315e-03  3.114e-04   7.432 1.13e-13 ***
entropy_Density                1.460e+01  3.838e+00   3.803 0.000143 ***
wtd_entropy_Density           -1.744e+01  2.458e+00  -7.094 1.36e-12 ***
range_Density                 -1.761e-03  2.534e-04  -6.949 3.82e-12 ***
std_Density                    6.392e-03  7.734e-04   8.264  < 2e-16 ***
wtd_std_Density               -1.466e-03  4.567e-04  -3.209 0.001333 **
wtd_mean_ElectronAffinity      4.402e-01  4.156e-02  10.590  < 2e-16 ***
gmean_ElectronAffinity         8.096e-02  2.059e-02   3.931 8.49e-05 ***
wtd_gmean_ElectronAffinity    -4.925e-01  3.998e-02 -12.318  < 2e-16 ***
entropy_ElectronAffinity       5.481e+00  3.065e+00   1.788 0.073760 .
wtd_entropy_ElectronAffinity  -2.467e+01  2.557e+00  -9.651  < 2e-16 ***
range_ElectronAffinity        -3.805e-01  2.055e-02 -18.520  < 2e-16 ***
```

```
wtd_range_ElectronAffinity      -1.620e-01  2.329e-02  -6.954 3.69e-12 ***
std_ElectronAffinity             1.205e+00  6.334e-02  19.022  < 2e-16 ***
wtd_std_ElectronAffinity        -4.900e-01  3.848e-02 -12.734  < 2e-16 ***
mean_FusionHeat                  1.447e+00  1.656e-01   8.739  < 2e-16 ***
wtd_mean_FusionHeat             -1.683e+00  1.834e-01  -9.176  < 2e-16 ***
gmean_FusionHeat                -1.256e+00  1.622e-01  -7.741 1.05e-14 ***
wtd_gmean_FusionHeat             1.328e+00  1.792e-01   7.411 1.32e-13 ***
entropy_FusionHeat              -1.713e+01  3.047e+00  -5.624 1.90e-08 ***
wtd_entropy_FusionHeat           2.371e+01  2.069e+00  11.462  < 2e-16 ***
range_FusionHeat                -4.738e-01  4.754e-02  -9.966  < 2e-16 ***
wtd_range_FusionHeat             5.976e-01  6.774e-02   8.821  < 2e-16 ***
wtd_std_FusionHeat               4.295e-01  1.274e-01   3.371 0.000752 ***
mean_ThermalConductivity        -5.450e-02  2.627e-02  -2.075 0.038033 *
wtd_mean_ThermalConductivity     5.137e-01  2.402e-02  21.384  < 2e-16 ***
gmean_ThermalConductivity       -7.516e-02  2.276e-02  -3.302 0.000962 ***
wtd_gmean_ThermalConductivity   -3.105e-01  1.934e-02 -16.055  < 2e-16 ***
entropy_ThermalConductivity      1.062e+01  2.245e+00   4.731 2.26e-06 ***
wtd_entropy_ThermalConductivity  2.873e+00  1.685e+00   1.705 0.088274 .
range_ThermalConductivity       -9.749e-02  1.571e-02  -6.206 5.58e-10 ***
wtd_range_ThermalConductivity   -2.231e-01  1.877e-02 -11.891  < 2e-16 ***
std_ThermalConductivity          2.912e-01  4.458e-02   6.531 6.73e-11 ***
mean_Valence                    -1.532e+01  6.901e+00  -2.219 0.026486 *
wtd_mean_Valence                 2.665e+01  7.989e+00   3.336 0.000853 ***
gmean_Valence                    1.966e+01  6.563e+00   2.995 0.002749 **
wtd_gmean_Valence               -3.119e+01  7.580e+00  -4.114 3.91e-05 ***
entropy_Valence                  8.363e+01  1.412e+01   5.923 3.22e-09 ***
wtd_entropy_Valence             -6.315e+01  5.702e+00 -11.075  < 2e-16 ***
range_Valence                    5.845e+00  8.707e-01   6.713 1.97e-11 ***
std_Valence                      5.630e+00  2.798e+00   2.012 0.044238 *
wtd_std_Valence                 -2.699e+01  2.116e+00 -12.753  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.62 on 14813 degrees of freedom
Multiple R-squared:  0.7367,Adjusted R-squared:  0.7355
F-statistic: 592.2 on 70 and 14813 DF,  p-value: < 2.2e-16
```

[52]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.step.backward.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 70 predictors is been used"
```

[53]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.all.summary$adj.r.
 ↪squared,4)))
```

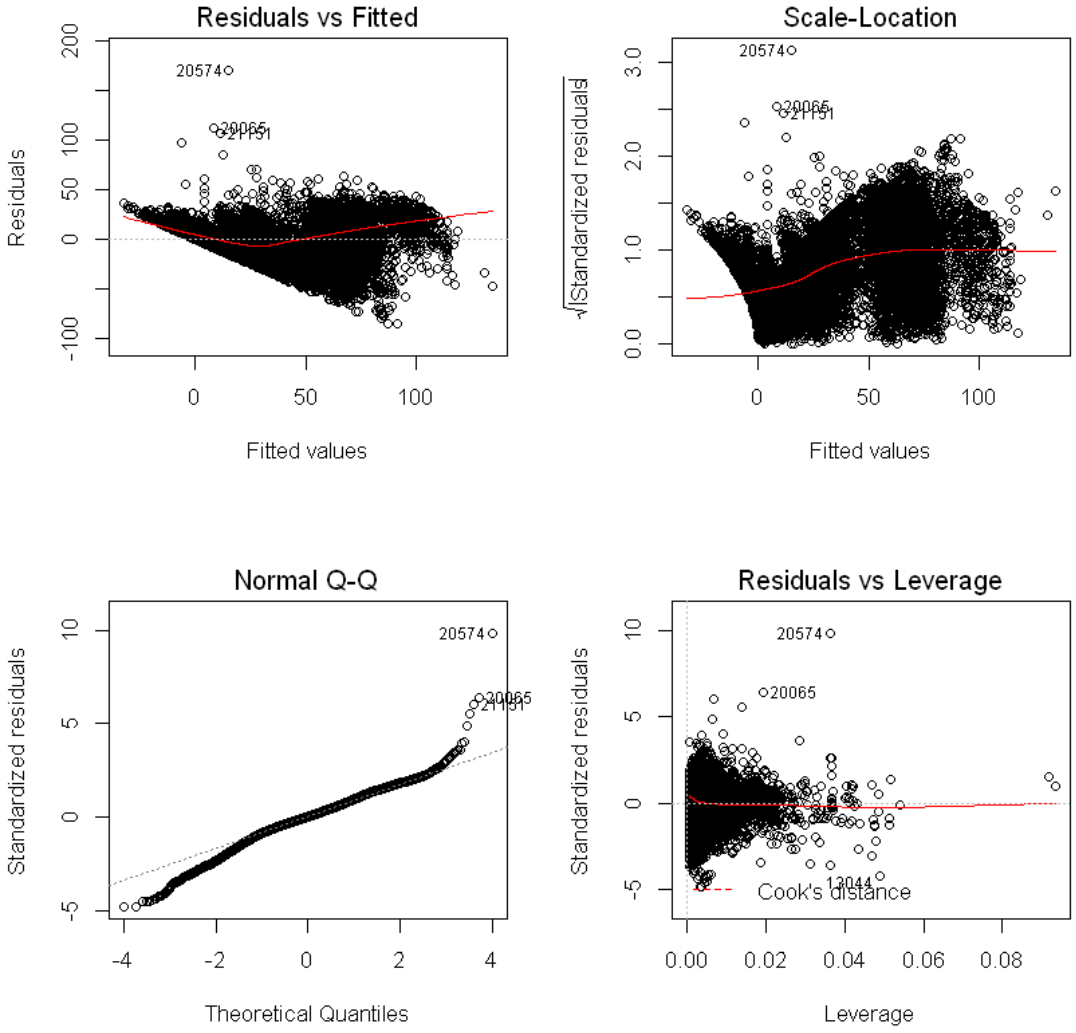
```
print(paste("Step Backward Data - Adjusted R-Square:",round(fit.step.backward.
 ↪summary$adj.r.squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7355"
[1] "Step Backward Data - Adjusted R-Square: 0.7355"
```

Here we can see that the adjusted R-square is almost equal which indicates that it might be a better model compared to original model(including all predicates) as this model is comparitively less complex

Lets Check the various Residuals plot

[54]:
```
par(mfcol=c(2,2))
plot(fit.step.backward)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.9 Perform F-tests by comparing the two models using the anova() function

[55]:
```
anova(fit.all, fit.step.backward)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14813	4598388	-11	-3488.991	1.021766	0.4234977

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are not much correlated as p value is greater than 0.05. we can also see that in the new fit the no of predictors is less compared to the original which makes it less complex. Also we can see that there is only slight increase in RSS compared to the original fit. So due to all these factors the new model looks better than the all predictors model

We Know that step is done by finding least AIC value. But a better model can also be found using other factors similar to AIC like BIC etc

4.1.10 Performing best subset selection

4.1.11 Using forward Selection

[56]:
```
fit.reg.forward <- regsubsets(critical_temp ~ ., data = train, nvmax = 81,␣
 ↪method = "forward")
fit.reg.forward.summary <- summary(fit.reg.forward)
fit.reg.forward.summary
```

```
Subset selection object
Call: regsubsets.formula(critical_temp ~ ., data = train, nvmax = 81,
    method = "forward")
81 Variables  (and intercept)
                              Forced in Forced out
number_of_elements                FALSE      FALSE
mean_atomic_mass                  FALSE      FALSE
wtd_mean_atomic_mass              FALSE      FALSE
gmean_atomic_mass                 FALSE      FALSE
wtd_gmean_atomic_mass             FALSE      FALSE
entropy_atomic_mass               FALSE      FALSE
wtd_entropy_atomic_mass           FALSE      FALSE
range_atomic_mass                 FALSE      FALSE
wtd_range_atomic_mass             FALSE      FALSE
std_atomic_mass                   FALSE      FALSE
wtd_std_atomic_mass               FALSE      FALSE
mean_fie                          FALSE      FALSE
wtd_mean_fie                      FALSE      FALSE
gmean_fie                         FALSE      FALSE
wtd_gmean_fie                     FALSE      FALSE
entropy_fie                       FALSE      FALSE
wtd_entropy_fie                   FALSE      FALSE
range_fie                         FALSE      FALSE
wtd_range_fie                     FALSE      FALSE
std_fie                           FALSE      FALSE
wtd_std_fie                       FALSE      FALSE
mean_atomic_radius                FALSE      FALSE
wtd_mean_atomic_radius            FALSE      FALSE
gmean_atomic_radius               FALSE      FALSE
wtd_gmean_atomic_radius           FALSE      FALSE
entropy_atomic_radius             FALSE      FALSE
wtd_entropy_atomic_radius         FALSE      FALSE
range_atomic_radius               FALSE      FALSE
wtd_range_atomic_radius           FALSE      FALSE
std_atomic_radius                 FALSE      FALSE
wtd_std_atomic_radius             FALSE      FALSE
mean_Density                      FALSE      FALSE
wtd_mean_Density                  FALSE      FALSE
gmean_Density                     FALSE      FALSE
```

```
wtd_gmean_Density                   FALSE      FALSE
entropy_Density                     FALSE      FALSE
wtd_entropy_Density                 FALSE      FALSE
range_Density                       FALSE      FALSE
wtd_range_Density                   FALSE      FALSE
std_Density                         FALSE      FALSE
wtd_std_Density                     FALSE      FALSE
mean_ElectronAffinity               FALSE      FALSE
wtd_mean_ElectronAffinity           FALSE      FALSE
gmean_ElectronAffinity              FALSE      FALSE
wtd_gmean_ElectronAffinity          FALSE      FALSE
entropy_ElectronAffinity            FALSE      FALSE
wtd_entropy_ElectronAffinity        FALSE      FALSE
range_ElectronAffinity              FALSE      FALSE
wtd_range_ElectronAffinity          FALSE      FALSE
std_ElectronAffinity                FALSE      FALSE
wtd_std_ElectronAffinity            FALSE      FALSE
mean_FusionHeat                     FALSE      FALSE
wtd_mean_FusionHeat                 FALSE      FALSE
gmean_FusionHeat                    FALSE      FALSE
wtd_gmean_FusionHeat                FALSE      FALSE
entropy_FusionHeat                  FALSE      FALSE
wtd_entropy_FusionHeat              FALSE      FALSE
range_FusionHeat                    FALSE      FALSE
wtd_range_FusionHeat                FALSE      FALSE
std_FusionHeat                      FALSE      FALSE
wtd_std_FusionHeat                  FALSE      FALSE
mean_ThermalConductivity            FALSE      FALSE
wtd_mean_ThermalConductivity        FALSE      FALSE
gmean_ThermalConductivity           FALSE      FALSE
wtd_gmean_ThermalConductivity       FALSE      FALSE
entropy_ThermalConductivity         FALSE      FALSE
wtd_entropy_ThermalConductivity     FALSE      FALSE
range_ThermalConductivity           FALSE      FALSE
wtd_range_ThermalConductivity       FALSE      FALSE
std_ThermalConductivity             FALSE      FALSE
wtd_std_ThermalConductivity         FALSE      FALSE
mean_Valence                        FALSE      FALSE
wtd_mean_Valence                    FALSE      FALSE
gmean_Valence                       FALSE      FALSE
wtd_gmean_Valence                   FALSE      FALSE
entropy_Valence                     FALSE      FALSE
wtd_entropy_Valence                 FALSE      FALSE
range_Valence                       FALSE      FALSE
wtd_range_Valence                   FALSE      FALSE
std_Valence                         FALSE      FALSE
wtd_std_Valence                     FALSE      FALSE
1 subsets of each size up to 81
```

```
Selection Algorithm: forward
          number_of_elements mean_atomic_mass wtd_mean_atomic_mass
1  ( 1 )  " "                " "              " "
2  ( 1 )  " "                " "              " "
3  ( 1 )  " "                " "              " "
4  ( 1 )  " "                " "              " "
5  ( 1 )  " "                " "              " "
6  ( 1 )  " "                " "              " "
7  ( 1 )  " "                " "              " "
8  ( 1 )  " "                " "              " "
9  ( 1 )  " "                " "              " "
10  ( 1 ) " "                " "              " "
11  ( 1 ) " "                " "              " "
12  ( 1 ) " "                " "              " "
13  ( 1 ) " "                " "              " "
14  ( 1 ) " "                " "              " "
15  ( 1 ) " "                " "              " "
16  ( 1 ) " "                " "              " "
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18  ( 1 ) " "                " "              " "
19  ( 1 ) " "                " "              " "
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31  ( 1 ) " "                " "              " "
32  ( 1 ) " "                " "              " "
33  ( 1 ) " "                " "              " "
34  ( 1 ) " "                " "              " "
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38  ( 1 ) " "                " "              " "
39  ( 1 ) " "                " "              " "
40  ( 1 ) " "                "*"              " "
41  ( 1 ) " "                "*"              " "
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43  ( 1 ) " "                "*"              "*"
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46  ( 1 ) " "                "*"              "*"
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47  ( 1 ) " "                "*"              "*"
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78  ( 1 ) "*"                "*"              "*"
79  ( 1 ) "*"                "*"              "*"
80  ( 1 ) "*"                "*"              "*"
81  ( 1 ) "*"                "*"              "*"
          gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
1   ( 1 )  " "               " "                  " "
2   ( 1 )  " "               " "                  " "
3   ( 1 )  " "               " "                  " "
4   ( 1 )  " "               " "                  " "
5   ( 1 )  " "               " "                  " "
6   ( 1 )  " "               " "                  " "
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9   ( 1 )  " "               " "                  " "
10   ( 1 ) " "               " "                  " "
11   ( 1 ) " "               " "                  " "
12   ( 1 ) " "               " "                  " "
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13  ( 1 ) " "               " "                 " "
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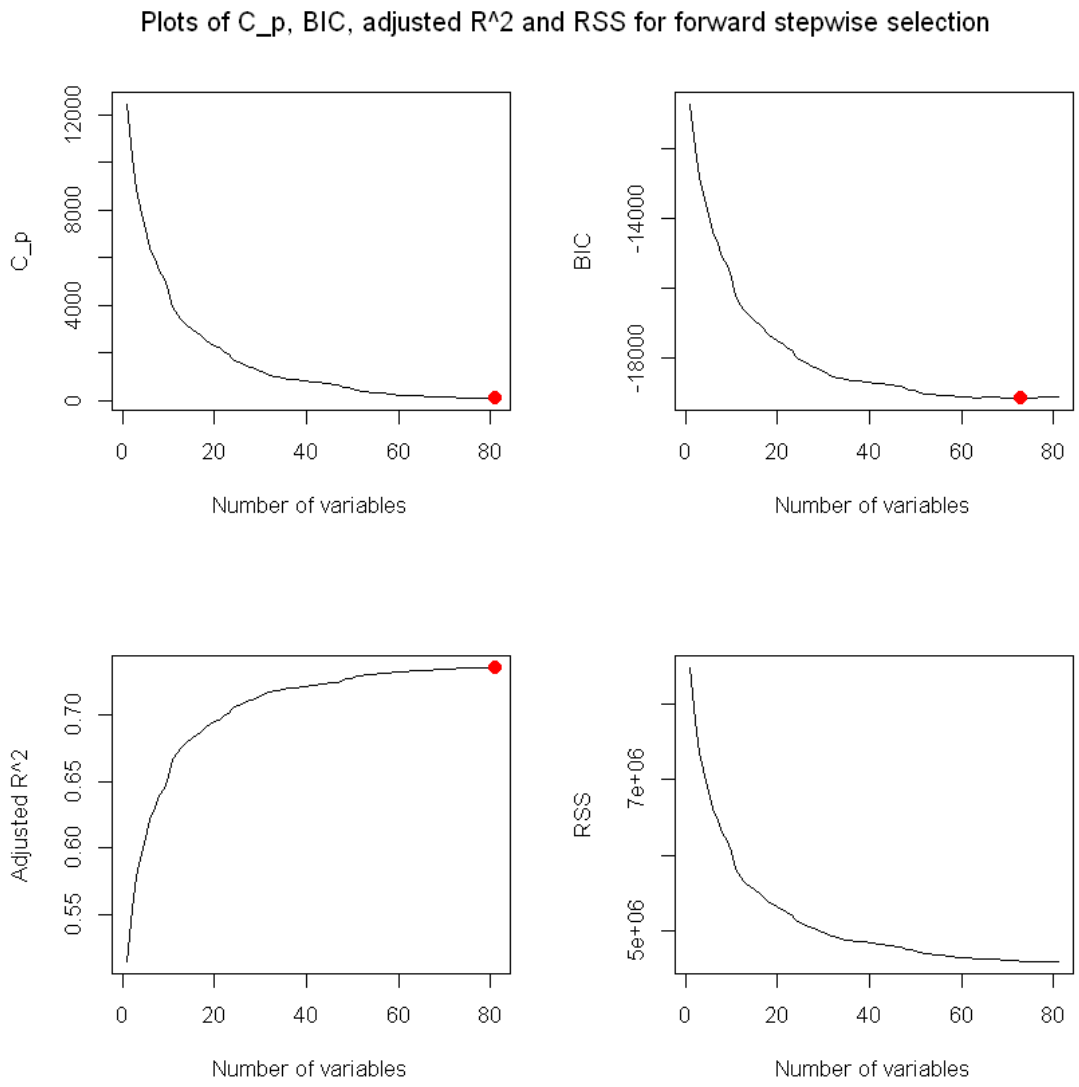
[57]:
```
par(mfrow = c(2, 2))
plot(fit.reg.forward.summary$cp, xlab = "Number of variables", ylab = "C_p",␣
 ↪type = "l")
points(which.min(fit.reg.forward.summary$cp), fit.reg.forward.summary$cp[which.
 ↪min(fit.reg.forward.summary$cp)], col = "red", cex = 2, pch = 20)
plot(fit.reg.forward.summary$bic, xlab = "Number of variables", ylab = "BIC",␣
 ↪type = "l")
points(which.min(fit.reg.forward.summary$bic), fit.reg.forward.
 ↪summary$bic[which.min(fit.reg.forward.summary$bic)], col = "red", cex = 2,␣
 ↪pch = 20)
plot(fit.reg.forward.summary$adjr2, xlab = "Number of variables", ylab =␣
 ↪"Adjusted R^2", type = "l")
points(which.max(fit.reg.forward.summary$adjr2), fit.reg.forward.
 ↪summary$adjr2[which.max(fit.reg.forward.summary$adjr2)], col = "red", cex =␣
 ↪2, pch = 20)
plot(fit.reg.forward.summary$rss, xlab = "Number of variables", ylab = "RSS",␣
 ↪type = "l")
mtext("Plots of C_p, BIC, adjusted R^2 and RSS for forward stepwise selection",␣
 ↪side = 3, line = -2, outer = TRUE)
```



BIC (or Bayesian information criteria) is a variant of AIC with a stronger penalty for including additional variables to the model.We know that lesser the value of BIC better the model

[58]:
```
print(paste("we can see that min value of BIC was found in a model with", which.
 ↪min(fit.reg.forward.summary$bic),"predictors"))
```

```
[1] "we can see that min value of BIC was found in a model with 73 predictors"
```

We also know that bigger the value of adjusted R square better the model

[59]:
```
print(paste("we can see that max value of Adjusted R Square was found in a␣
 ↪model with",
            which.max(fit.reg.forward.summary$adjr2),"predictors"))
```

```
[1] "we can see that max value of Adjusted R Square was found in a model with 81
predictors"
```

Mallows Cp: A variant of AIC developed by Colin Mallows. We also Know that the smaller the value of Cp better the model

[60]:
```
print(paste("we can see that max value of Cp was found in a model with", which.
↪min(fit.reg.forward.summary$cp),"predictors"))
```

```
[1] "we can see that max value of Cp was found in a model with 81 predictors"
```

Here we can see that based on both Cp and Adjusted R2 the best model should have 81 predicates. Which is same as the all predictors model

So lets analyse the case with lowet BIC that is the model with 73 predictors

[61]:
```
fBicSelectedColumns = names(coef(fit.reg.forward,73))
# Chang in the value of '(Intercept) to critical_temp
fBicSelectedColumns[1] = 'critical_temp'
fBicSelectedColumns
```

1. 'critical_temp' 2. 'number_of_elements' 3. 'mean_atomic_mass' 4. 'wtd_mean_atomic_mass' 5. 'gmean_atomic_mass' 6. 'wtd_gmean_atomic_mass' 7. 'entropy_atomic_mass' 8. 'wtd_entropy_atomic_mass' 9. 'range_atomic_mass' 10. 'std_atomic_mass' 11. 'wtd_std_atomic_mass' 12. 'wtd_gmean_fie' 13. 'entropy_fie' 14. 'wtd_entropy_fie' 15. 'range_fie' 16. 'wtd_range_fie' 17. 'std_fie' 18. 'wtd_std_fie' 19. 'wtd_mean_atomic_radius' 20. 'gmean_atomic_radius' 21. 'wtd_gmean_atomic_radius' 22. 'entropy_atomic_radius' 23. 'wtd_entropy_atomic_radius' 24. 'range_atomic_radius' 25. 'wtd_range_atomic_radius' 26. 'std_atomic_radius' 27. 'wtd_std_atomic_radius' 28. 'mean_Density' 29. 'wtd_mean_Density' 30. 'gmean_Density' 31. 'wtd_gmean_Density' 32. 'entropy_Density' 33. 'wtd_entropy_Density' 34. 'range_Density' 35. 'wtd_range_Density' 36. 'std_Density' 37. 'wtd_std_Density' 38. 'mean_ElectronAffinity' 39. 'wtd_mean_ElectronAffinity' 40. 'gmean_ElectronAffinity' 41. 'wtd_gmean_ElectronAffinity' 42. 'entropy_ElectronAffinity' 43. 'wtd_entropy_ElectronAffinity' 44. 'range_ElectronAffinity' 45. 'wtd_range_ElectronAffinity' 46. 'std_ElectronAffinity' 47. 'wtd_std_ElectronAffinity' 48. 'mean_FusionHeat' 49. 'wtd_mean_FusionHeat' 50. 'gmean_FusionHeat' 51. 'wtd_gmean_FusionHeat' 52. 'entropy_FusionHeat' 53. 'wtd_entropy_FusionHeat' 54. 'range_FusionHeat' 55. 'wtd_range_FusionHeat' 56. 'std_FusionHeat' 57. 'wtd_std_FusionHeat' 58. 'mean_ThermalConductivity' 59. 'wtd_mean_ThermalConductivity' 60. 'gmean_ThermalConductivity' 61. 'wtd_gmean_ThermalConductivity' 62. 'entropy_ThermalConductivity' 63. 'wtd_entropy_ThermalConductivity' 64. 'range_ThermalConductivity' 65. 'wtd_range_ThermalConductivity' 66. 'std_ThermalConductivity' 67. 'wtd_std_ThermalConductivity' 68. 'gmean_Valence' 69. 'wtd_gmean_Valence' 70. 'entropy_Valence' 71. 'wtd_entropy_Valence' 72. 'range_Valence' 73. 'wtd_range_Valence' 74. 'wtd_std_Valence'

[62]:
```
fBicTrain = train[,fBicSelectedColumns]
head(fBicTrain)
```

	critical_temp	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atc
18847	24.0	6	60.60051	71.50999	46.72851
18895	15.5	4	57.44445	60.35930	56.06791
2986	45.3	6	84.71115	78.84015	66.61372
1842	94.0	7	112.95469	60.86673	82.42970
3371	74.1	6	78.67813	59.21927	58.87964
11638	12.9	3	49.59452	37.84410	37.11177

[63]:
```
fit.reg.f.bic = lm(critical_temp~., data = fBicTrain)
fit.reg.f.bic.summary = summary(fit.reg.f.bic)
fit.reg.f.bic.summary
```

```
Call:
lm(formula = critical_temp ~ ., data = fBicTrain)

Residuals:
   Min     1Q Median     3Q    Max
-84.10  -9.36   0.52  10.82 169.94

Coefficients:
                                Estimate Std. Error t value Pr(>|t|)
(Intercept)                   -2.559e+01  5.491e+00  -4.661 3.18e-06 ***
number_of_elements            -2.875e+00  8.824e-01  -3.258 0.001123 **
mean_atomic_mass               7.188e-01  9.527e-02   7.544 4.82e-14 ***
wtd_mean_atomic_mass          -6.917e-01  1.177e-01  -5.875 4.33e-09 ***
gmean_atomic_mass             -3.679e-01  9.345e-02  -3.937 8.29e-05 ***
wtd_gmean_atomic_mass          4.410e-01  1.118e-01   3.944 8.05e-05 ***
entropy_atomic_mass           -3.843e+01  5.267e+00  -7.296 3.11e-13 ***
wtd_entropy_atomic_mass        3.554e+00  3.899e+00   0.912 0.362043
range_atomic_mass              2.130e-01  1.939e-02  10.984  < 2e-16 ***
std_atomic_mass               -5.076e-01  7.269e-02  -6.983 3.02e-12 ***
wtd_std_atomic_mass            1.630e-02  6.198e-02   0.263 0.792532
wtd_gmean_fie                  3.067e-02  4.884e-03   6.280 3.47e-10 ***
entropy_fie                   -1.059e+02  1.998e+01  -5.299 1.18e-07 ***
wtd_entropy_fie                5.374e+01  5.078e+00  10.583  < 2e-16 ***
range_fie                      6.622e-02  7.665e-03   8.638  < 2e-16 ***
wtd_range_fie                  2.348e-02  4.235e-03   5.545 2.98e-08 ***
std_fie                       -1.580e-01  1.979e-02  -7.986 1.49e-15 ***
wtd_std_fie                   -5.719e-02  1.118e-02  -5.115 3.18e-07 ***
wtd_mean_atomic_radius         2.542e+00  1.621e-01  15.678  < 2e-16 ***
gmean_atomic_radius           -3.434e-01  3.178e-02 -10.806  < 2e-16 ***
wtd_gmean_atomic_radius       -2.128e+00  1.557e-01 -13.670  < 2e-16 ***
entropy_atomic_radius          6.755e+01  1.854e+01   3.644 0.000269 ***
wtd_entropy_atomic_radius      4.329e+01  5.935e+00   7.294 3.16e-13 ***
range_atomic_radius            2.211e-01  2.599e-02   8.507  < 2e-16 ***
wtd_range_atomic_radius       -8.896e-02  1.759e-02  -5.057 4.32e-07 ***
std_atomic_radius             -6.110e-01  8.051e-02  -7.589 3.42e-14 ***
wtd_std_atomic_radius         -1.114e-01  7.073e-02  -1.575 0.115326
mean_Density                  -4.933e-03  5.853e-04  -8.428  < 2e-16 ***
wtd_mean_Density              -5.105e-04  6.961e-04  -0.733 0.463389
gmean_Density                  1.336e-03  5.457e-04   2.448 0.014363 *
wtd_gmean_Density              2.391e-03  6.669e-04   3.585 0.000338 ***
entropy_Density                1.588e+01  3.978e+00   3.992 6.59e-05 ***
wtd_entropy_Density           -1.649e+01  2.958e+00  -5.573 2.55e-08 ***
range_Density                 -1.628e-03  2.543e-04  -6.399 1.61e-10 ***
```

```
wtd_range_Density                3.427e-04  2.345e-04   1.462 0.143892
std_Density                      5.952e-03  8.127e-04   7.324 2.54e-13 ***
wtd_std_Density                 -1.232e-03  5.906e-04  -2.086 0.037022 *
mean_ElectronAffinity           -1.030e-01  5.312e-02  -1.938 0.052590 .
wtd_mean_ElectronAffinity        5.363e-01  5.820e-02   9.215  < 2e-16 ***
gmean_ElectronAffinity           1.574e-01  4.751e-02   3.314 0.000921 ***
wtd_gmean_ElectronAffinity      -5.648e-01  5.198e-02 -10.865  < 2e-16 ***
entropy_ElectronAffinity         5.230e+00  3.045e+00   1.717 0.085920 .
wtd_entropy_ElectronAffinity    -2.381e+01  2.622e+00  -9.082  < 2e-16 ***
range_ElectronAffinity          -3.847e-01  2.014e-02 -19.100  < 2e-16 ***
wtd_range_ElectronAffinity      -1.692e-01  2.468e-02  -6.857 7.33e-12 ***
std_ElectronAffinity             1.273e+00  6.781e-02  18.776  < 2e-16 ***
wtd_std_ElectronAffinity        -5.391e-01  4.605e-02 -11.708  < 2e-16 ***
mean_FusionHeat                  1.479e+00  2.188e-01   6.760 1.43e-11 ***
wtd_mean_FusionHeat             -1.748e+00  2.215e-01  -7.893 3.15e-15 ***
gmean_FusionHeat                -1.298e+00  1.997e-01  -6.501 8.22e-11 ***
wtd_gmean_FusionHeat             1.395e+00  2.053e-01   6.797 1.11e-11 ***
entropy_FusionHeat              -1.858e+01  3.209e+00  -5.791 7.13e-09 ***
wtd_entropy_FusionHeat           2.521e+01  2.277e+00  11.071  < 2e-16 ***
range_FusionHeat                -4.043e-01  7.868e-02  -5.139 2.80e-07 ***
wtd_range_FusionHeat             6.128e-01  7.956e-02   7.702 1.42e-14 ***
std_FusionHeat                  -2.964e-01  3.068e-01  -0.966 0.333981
wtd_std_FusionHeat               5.775e-01  1.771e-01   3.262 0.001110 **
mean_ThermalConductivity        -6.523e-02  2.899e-02  -2.250 0.024432 *
wtd_mean_ThermalConductivity     5.454e-01  3.184e-02  17.131  < 2e-16 ***
gmean_ThermalConductivity       -5.287e-02  2.720e-02  -1.944 0.051963 .
wtd_gmean_ThermalConductivity   -3.502e-01  3.033e-02 -11.545  < 2e-16 ***
entropy_ThermalConductivity      1.123e+01  2.339e+00   4.801 1.59e-06 ***
wtd_entropy_ThermalConductivity  1.565e+00  1.889e+00   0.829 0.407341
range_ThermalConductivity       -9.936e-02  1.573e-02  -6.317 2.75e-10 ***
wtd_range_ThermalConductivity   -2.235e-01  1.920e-02 -11.641  < 2e-16 ***
std_ThermalConductivity          3.122e-01  4.885e-02   6.392 1.69e-10 ***
wtd_std_ThermalConductivity     -2.949e-02  2.665e-02  -1.107 0.268521
gmean_Valence                    5.693e+00  9.566e-01   5.952 2.71e-09 ***
wtd_gmean_Valence               -5.577e+00  9.606e-01  -5.806 6.53e-09 ***
entropy_Valence                  7.206e+01  1.096e+01   6.573 5.08e-11 ***
wtd_entropy_Valence             -7.716e+01  5.608e+00 -13.759  < 2e-16 ***
range_Valence                    6.028e+00  4.958e-01  12.158  < 2e-16 ***
wtd_range_Valence               -5.556e-01  7.416e-01  -0.749 0.453778
wtd_std_Valence                 -2.036e+01  1.059e+00 -19.221  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.63 on 14810 degrees of freedom
Multiple R-squared:  0.7365,Adjusted R-squared:  0.7352
F-statistic: 567.2 on 73 and 14810 DF,  p-value: < 2.2e-16
```

[64]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.reg.f.bic.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 73 predictors is been used"
```

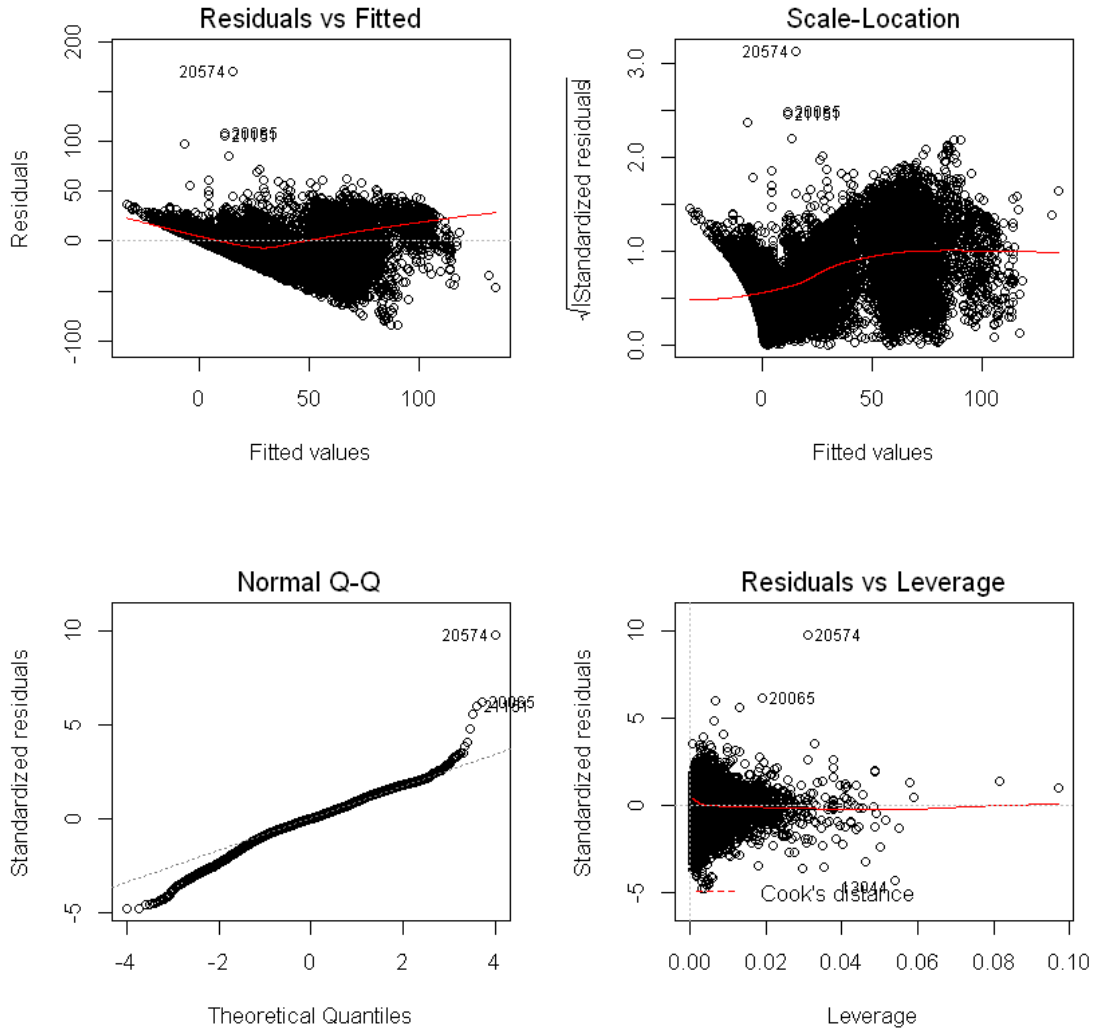
[65]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.reg.f.bic.
 ↪summary$adj.r.squared,4)))
print(paste("Based on Min BIC Val - Adjusted R-Square:",round(fit.reg.f.bic.
 ↪summary$adj.r.squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7352"
[1] "Based on Min BIC Val - Adjusted R-Square: 0.7352"
```

Here we can see that the adjusted R-square is decreased but only for a small amount which indicates that it might be a better model compared to original model(including all predicates) as this model is comparitively less complex

Lets Check the various Residuals plot

[66]:
```
par(mfcol=c(2,2))
plot(fit.reg.f.bic)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if

residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.12 Perform F-tests by comparing the two models using the anova() function

[67]:
```
anova(fit.all, fit.reg.f.bic)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14810	4601730	-8	-6831.795	2.750992	0.004923194

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are more correlated as p value is less than 0.05. we can also see that in the new fit the no of predictors is less compared to the original which makes it less complex. Also we can see that there is only slight increase in RSS compared to the original fit. So due to all these factors the new model looks better than the all predictors model

4.1.13 Using Backward Selection

[68]:
```
fit.reg.backward <- regsubsets(critical_temp ~ ., data = train, nvmax = 81,␣
 ↪method = "backward")
fit.reg.backward.summary <- summary(fit.reg.backward)
fit.reg.backward.summary
```

```
Subset selection object
Call: regsubsets.formula(critical_temp ~ ., data = train, nvmax = 81,
    method = "backward")
81 Variables  (and intercept)
                              Forced in Forced out
number_of_elements                FALSE      FALSE
mean_atomic_mass                  FALSE      FALSE
wtd_mean_atomic_mass              FALSE      FALSE
gmean_atomic_mass                 FALSE      FALSE
```

wtd_gmean_atomic_mass	FALSE	FALSE
entropy_atomic_mass	FALSE	FALSE
wtd_entropy_atomic_mass	FALSE	FALSE
range_atomic_mass	FALSE	FALSE
wtd_range_atomic_mass	FALSE	FALSE
std_atomic_mass	FALSE	FALSE
wtd_std_atomic_mass	FALSE	FALSE
mean_fie	FALSE	FALSE
wtd_mean_fie	FALSE	FALSE
gmean_fie	FALSE	FALSE
wtd_gmean_fie	FALSE	FALSE
entropy_fie	FALSE	FALSE
wtd_entropy_fie	FALSE	FALSE
range_fie	FALSE	FALSE
wtd_range_fie	FALSE	FALSE
std_fie	FALSE	FALSE
wtd_std_fie	FALSE	FALSE
mean_atomic_radius	FALSE	FALSE
wtd_mean_atomic_radius	FALSE	FALSE
gmean_atomic_radius	FALSE	FALSE
wtd_gmean_atomic_radius	FALSE	FALSE
entropy_atomic_radius	FALSE	FALSE
wtd_entropy_atomic_radius	FALSE	FALSE
range_atomic_radius	FALSE	FALSE
wtd_range_atomic_radius	FALSE	FALSE
std_atomic_radius	FALSE	FALSE
wtd_std_atomic_radius	FALSE	FALSE
mean_Density	FALSE	FALSE
wtd_mean_Density	FALSE	FALSE
gmean_Density	FALSE	FALSE
wtd_gmean_Density	FALSE	FALSE
entropy_Density	FALSE	FALSE
wtd_entropy_Density	FALSE	FALSE
range_Density	FALSE	FALSE
wtd_range_Density	FALSE	FALSE
std_Density	FALSE	FALSE
wtd_std_Density	FALSE	FALSE
mean_ElectronAffinity	FALSE	FALSE
wtd_mean_ElectronAffinity	FALSE	FALSE
gmean_ElectronAffinity	FALSE	FALSE
wtd_gmean_ElectronAffinity	FALSE	FALSE
entropy_ElectronAffinity	FALSE	FALSE
wtd_entropy_ElectronAffinity	FALSE	FALSE
range_ElectronAffinity	FALSE	FALSE
wtd_range_ElectronAffinity	FALSE	FALSE
std_ElectronAffinity	FALSE	FALSE
wtd_std_ElectronAffinity	FALSE	FALSE
mean_FusionHeat	FALSE	FALSE

```
wtd_mean_FusionHeat                FALSE      FALSE
gmean_FusionHeat                   FALSE      FALSE
wtd_gmean_FusionHeat               FALSE      FALSE
entropy_FusionHeat                 FALSE      FALSE
wtd_entropy_FusionHeat             FALSE      FALSE
range_FusionHeat                   FALSE      FALSE
wtd_range_FusionHeat               FALSE      FALSE
std_FusionHeat                     FALSE      FALSE
wtd_std_FusionHeat                 FALSE      FALSE
mean_ThermalConductivity           FALSE      FALSE
wtd_mean_ThermalConductivity       FALSE      FALSE
gmean_ThermalConductivity          FALSE      FALSE
wtd_gmean_ThermalConductivity      FALSE      FALSE
entropy_ThermalConductivity        FALSE      FALSE
wtd_entropy_ThermalConductivity    FALSE      FALSE
range_ThermalConductivity          FALSE      FALSE
wtd_range_ThermalConductivity      FALSE      FALSE
std_ThermalConductivity            FALSE      FALSE
wtd_std_ThermalConductivity        FALSE      FALSE
mean_Valence                       FALSE      FALSE
wtd_mean_Valence                   FALSE      FALSE
gmean_Valence                      FALSE      FALSE
wtd_gmean_Valence                  FALSE      FALSE
entropy_Valence                    FALSE      FALSE
wtd_entropy_Valence                FALSE      FALSE
range_Valence                      FALSE      FALSE
wtd_range_Valence                  FALSE      FALSE
std_Valence                        FALSE      FALSE
wtd_std_Valence                    FALSE      FALSE
1 subsets of each size up to 81
Selection Algorithm: backward
          number_of_elements mean_atomic_mass wtd_mean_atomic_mass
1  ( 1 )  " "                " "              " "
2  ( 1 )  " "                " "              " "
3  ( 1 )  " "                " "              " "
4  ( 1 )  " "                " "              " "
5  ( 1 )  " "                " "              " "
6  ( 1 )  " "                " "              " "
7  ( 1 )  " "                " "              " "
8  ( 1 )  " "                " "              " "
9  ( 1 )  " "                " "              " "
10  ( 1 ) " "                " "              " "
11  ( 1 ) " "                " "              " "
12  ( 1 ) " "                " "              " "
13  ( 1 ) " "                " "              " "
14  ( 1 ) " "                " "              " "
15  ( 1 ) " "                " "              " "
16  ( 1 ) " "                " "              " "
```

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17  ( 1 ) " "               " "             "*"
18  ( 1 ) " "               " "             "*"
19  ( 1 ) " "               " "             "*"
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63  ( 1 ) "*"               "*"             "*"
64  ( 1 ) "*"               "*"             "*"
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65  ( 1 ) "*"                "*"                "*"
66  ( 1 ) "*"                "*"                "*"
67  ( 1 ) "*"                "*"                "*"
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69  ( 1 ) "*"                "*"                "*"
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71  ( 1 ) "*"                "*"                "*"
72  ( 1 ) "*"                "*"                "*"
73  ( 1 ) "*"                "*"                "*"
74  ( 1 ) "*"                "*"                "*"
75  ( 1 ) "*"                "*"                "*"
76  ( 1 ) "*"                "*"                "*"
77  ( 1 ) "*"                "*"                "*"
78  ( 1 ) "*"                "*"                "*"
79  ( 1 ) "*"                "*"                "*"
80  ( 1 ) "*"                "*"                "*"
81  ( 1 ) "*"                "*"                "*"
          gmean_atomic_mass wtd_gmean_atomic_mass entropy_atomic_mass
1   ( 1 )  " "               " "                  " "
2   ( 1 )  " "               " "                  " "
3   ( 1 )  " "               " "                  " "
4   ( 1 )  " "               " "                  " "
5   ( 1 )  " "               " "                  " "
6   ( 1 )  " "               " "                  " "
7   ( 1 )  " "               " "                  " "
8   ( 1 )  " "               " "                  " "
9   ( 1 )  " "               " "                  " "
10  ( 1 ) " "                " "                  " "
11  ( 1 ) " "                " "                  " "
12  ( 1 ) " "                " "                  " "
13  ( 1 ) " "                " "                  " "
14  ( 1 ) " "                " "                  " "
15  ( 1 ) " "                " "                  " "
16  ( 1 ) " "                " "                  " "
17  ( 1 ) " "                " "                  " "
18  ( 1 ) " "                "*"                  " "
19  ( 1 ) " "                "*"                  "*"
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21  ( 1 ) " "                "*"                  "*"
22  ( 1 ) " "                "*"                  "*"
23  ( 1 ) " "                "*"                  "*"
24  ( 1 ) " "                "*"                  "*"
25  ( 1 ) " "                "*"                  "*"
26  ( 1 ) " "                "*"                  "*"
27  ( 1 ) " "                "*"                  "*"
28  ( 1 ) " "                "*"                  "*"
29  ( 1 ) " "                "*"                  "*"
30  ( 1 ) " "                "*"                  "*"
```

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31  ( 1 ) " "               "*"                 "*"
32  ( 1 ) " "               "*"                 "*"
33  ( 1 ) " "               "*"                 "*"
34  ( 1 ) " "               "*"                 "*"
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[69]:
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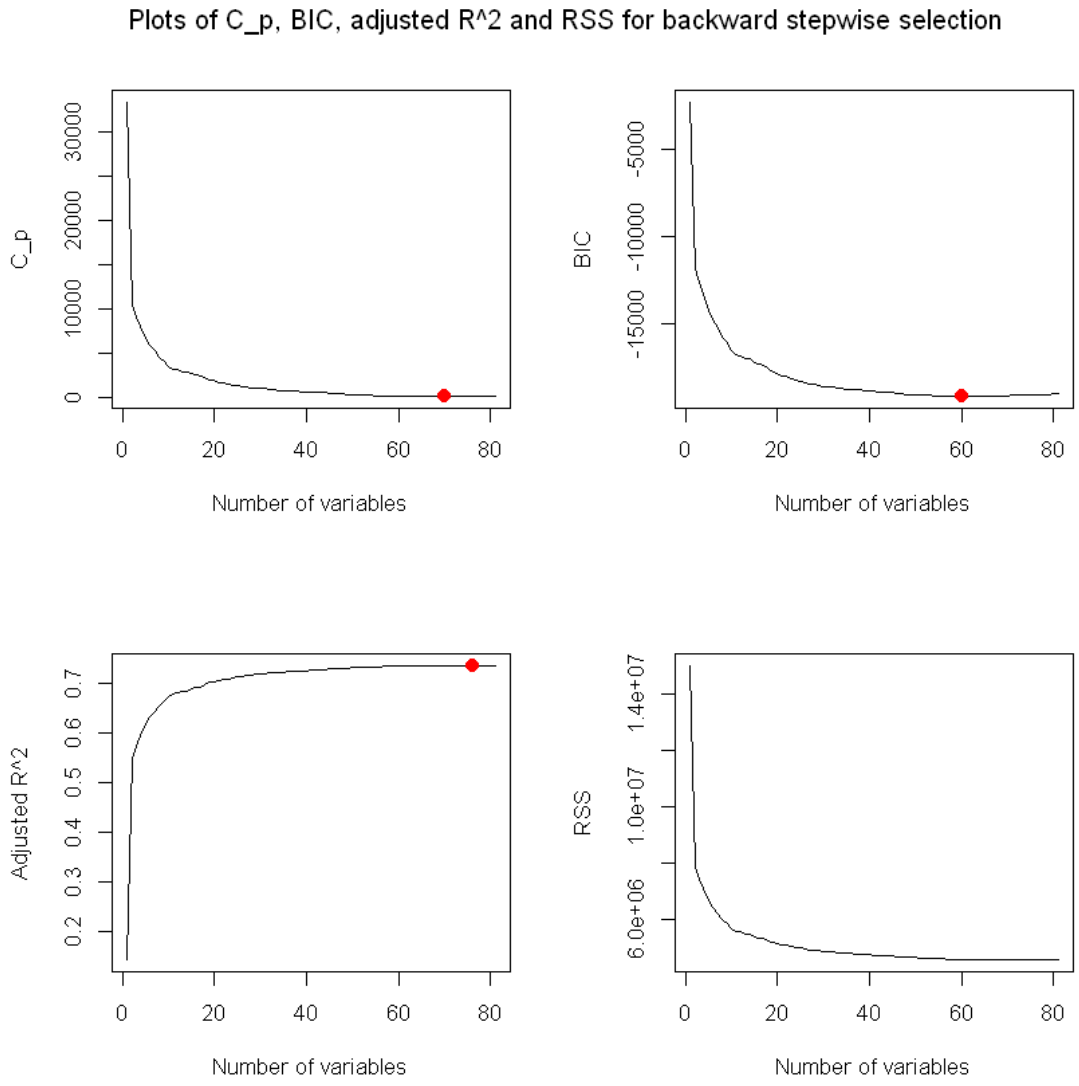
par(mfrow = c(2, 2))
plot(fit.reg.backward.summary$cp, xlab = "Number of variables", ylab = "C_p",␣
 ↪type = "l")
points(which.min(fit.reg.backward.summary$cp), fit.reg.backward.
 ↪summary$cp[which.min(fit.reg.backward.summary$cp)], col = "red", cex = 2,␣
 ↪pch = 20)
plot(fit.reg.backward.summary$bic, xlab = "Number of variables", ylab = "BIC",␣
 ↪type = "l")
```

```
points(which.min(fit.reg.backward.summary$bic), fit.reg.backward.
 ↪summary$bic[which.min(fit.reg.backward.summary$bic)], col = "red", cex = 2,␣
 ↪pch = 20)
plot(fit.reg.backward.summary$adjr2, xlab = "Number of variables", ylab =␣
 ↪"Adjusted R^2", type = "l")
points(which.max(fit.reg.backward.summary$adjr2), fit.reg.backward.
 ↪summary$adjr2[which.max(fit.reg.backward.summary$adjr2)], col = "red", cex =␣
 ↪2, pch = 20)
plot(fit.reg.backward.summary$rss, xlab = "Number of variables", ylab = "RSS",␣
 ↪type = "l")
mtext("Plots of C_p, BIC, adjusted R^2 and RSS for backward stepwise␣
 ↪selection", side = 3, line = -2, outer = TRUE)
```



BIC (or Bayesian information criteria) is a variant of AIC with a stronger penalty for including additional variables to the model.We know that lesser the value of BIC better the model

[70]:
```
print(paste("we can see that min value of BIC was found in a model with", which.
↪min(fit.reg.backward.summary$bic),"predictors"))
```

```
[1] "we can see that min value of BIC was found in a model with 60 predictors"
```

We also know that bigger the value of adjusted R square better the model

[71]:
```
print(paste("we can see that max value of Adjusted R Square was found in a␣
↪model with",
            which.max(fit.reg.backward.summary$adjr2),"predictors"))
```

```
[1] "we can see that max value of Adjusted R Square was found in a model with 76
predictors"
```

Mallows Cp: A variant of AIC developed by Colin Mallows. We also Know that the smaller the value of Cp better the model

[72]:
```
print(paste("we can see that max value of Cp was found in a model with", which.
↪min(fit.reg.backward.summary$cp),"predictors"))
```

```
[1] "we can see that max value of Cp was found in a model with 70 predictors"
```

Here we can see that all of them have different no of predictors. So lets start from analysing the best model based on BIC ie 60 predictors

based on BIC

[73]:
```
bBicSelectedColumns = names(coef(fit.reg.backward,60))
# Chang in the value of '(Intercept) to critical_temp
bBicSelectedColumns[1] = 'critical_temp'
bBicSelectedColumns
```

1. 'critical_temp' 2. 'number_of_elements' 3. 'mean_atomic_mass' 4. 'wtd_mean_atomic_mass' 5. 'gmean_atomic_mass' 6. 'wtd_gmean_atomic_mass' 7. 'entropy_atomic_mass' 8. 'range_atomic_mass' 9. 'std_atomic_mass' 10. 'mean_fie' 11. 'wtd_mean_fie' 12. 'gmean_fie' 13. 'wtd_gmean_fie' 14. 'entropy_fie' 15. 'wtd_entropy_fie' 16. 'range_fie' 17. 'wtd_range_fie' 18. 'std_fie' 19. 'mean_atomic_radius' 20. 'wtd_mean_atomic_radius' 21. 'wtd_gmean_atomic_radius' 22. 'entropy_atomic_radius' 23. 'wtd_entropy_atomic_radius' 24. 'range_atomic_radius' 25. 'wtd_range_atomic_radius' 26. 'std_atomic_radius' 27. 'mean_Density' 28. 'wtd_gmean_Density' 29. 'entropy_Density' 30. 'wtd_entropy_Density' 31. 'range_Density' 32. 'std_Density' 33. 'wtd_mean_ElectronAffinity' 34. 'gmean_ElectronAffinity' 35. 'wtd_gmean_ElectronAffinity' 36. 'wtd_entropy_ElectronAffinity' 37. 'range_ElectronAffinity' 38. 'wtd_range_ElectronAffinity' 39. 'std_ElectronAffinity' 40. 'wtd_std_ElectronAffinity' 41. 'mean_FusionHeat' 42. 'wtd_mean_FusionHeat' 43. 'gmean_FusionHeat' 44. 'wtd_gmean_FusionHeat' 45. 'entropy_FusionHeat' 46. 'wtd_entropy_FusionHeat' 47. 'range_FusionHeat' 48. 'wtd_range_FusionHeat' 49. 'wtd_mean_ThermalConductivity' 50. 'gmean_ThermalConductivity' 51. 'wtd_gmean_ThermalConductivity' 52. 'entropy_ThermalConductivity' 53. 'range_ThermalConductivity'

54. 'wtd_range_ThermalConductivity' 55. 'std_ThermalConductivity' 56. 'gmean_Valence' 57. 'wtd_gmean_Valence' 58. 'entropy_Valence' 59. 'wtd_entropy_Valence' 60. 'range_Valence' 61. 'wtd_std_Valence'

[74]:
```
bBicTrain = train[,bBicSelectedColumns]
head(bBicTrain)
```

	critical_temp	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_ato
18847	24.0	6	60.60051	71.50999	46.72851
18895	15.5	4	57.44445	60.35930	56.06791
2986	45.3	6	84.71115	78.84015	66.61372
1842	94.0	7	112.95469	60.86673	82.42970
3371	74.1	6	78.67813	59.21927	58.87964
11638	12.9	3	49.59452	37.84410	37.11177

[75]:
```
fit.reg.b.bic = lm(critical_temp~., data = bBicTrain)
fit.reg.b.bic.summary = summary(fit.reg.b.bic)
fit.reg.b.bic.summary
```

```
Call:
lm(formula = critical_temp ~ ., data = bBicTrain)

Residuals:
    Min      1Q  Median      3Q     Max
-84.157  -9.440   0.561  10.958 173.433

Coefficients:
                            Estimate Std. Error t value Pr(>|t|)
(Intercept)               -1.899e+01  5.708e+00  -3.327 0.000880 ***
number_of_elements        -3.485e+00  8.522e-01  -4.090 4.33e-05 ***
mean_atomic_mass           8.318e-01  6.316e-02  13.169  < 2e-16 ***
wtd_mean_atomic_mass      -8.596e-01  5.118e-02 -16.795  < 2e-16 ***
gmean_atomic_mass         -4.434e-01  6.567e-02  -6.752 1.51e-11 ***
wtd_gmean_atomic_mass      5.653e-01  5.627e-02  10.046  < 2e-16 ***
entropy_atomic_mass       -3.705e+01  4.712e+00  -7.862 4.03e-15 ***
range_atomic_mass          2.138e-01  1.903e-02  11.233  < 2e-16 ***
std_atomic_mass           -4.936e-01  5.156e-02  -9.575  < 2e-16 ***
mean_fie                   2.576e-01  4.801e-02   5.365 8.22e-08 ***
wtd_mean_fie              -2.937e-01  3.998e-02  -7.346 2.14e-13 ***
gmean_fie                 -2.589e-01  4.753e-02  -5.447 5.20e-08 ***
wtd_gmean_fie              3.171e-01  4.038e-02   7.854 4.31e-15 ***
entropy_fie               -1.032e+02  2.098e+01  -4.918 8.86e-07 ***
wtd_entropy_fie            5.068e+01  4.661e+00  10.873  < 2e-16 ***
range_fie                  7.046e-02  7.443e-03   9.468  < 2e-16 ***
wtd_range_fie              2.171e-02  3.760e-03   5.772 7.98e-09 ***
std_fie                   -2.165e-01  1.911e-02 -11.330  < 2e-16 ***
mean_atomic_radius        -3.085e-01  2.928e-02 -10.535  < 2e-16 ***
wtd_mean_atomic_radius     2.616e+00  1.195e-01  21.881  < 2e-16 ***
wtd_gmean_atomic_radius   -2.243e+00  1.168e-01 -19.206  < 2e-16 ***
entropy_atomic_radius      5.822e+01  1.878e+01   3.101 0.001934 **
```

```
wtd_entropy_atomic_radius      4.791e+01  4.297e+00  11.150  < 2e-16 ***
range_atomic_radius            2.009e-01  2.559e-02   7.852 4.37e-15 ***
wtd_range_atomic_radius       -7.278e-02  1.403e-02  -5.189 2.15e-07 ***
std_atomic_radius             -6.128e-01  6.690e-02  -9.161  < 2e-16 ***
mean_Density                  -4.480e-03  3.009e-04 -14.891  < 2e-16 ***
wtd_gmean_Density              3.059e-03  2.659e-04  11.506  < 2e-16 ***
entropy_Density                1.196e+01  3.521e+00   3.396 0.000684 ***
wtd_entropy_Density           -1.550e+01  2.183e+00  -7.102 1.28e-12 ***
range_Density                 -1.643e-03  2.489e-04  -6.601 4.22e-11 ***
std_Density                    4.645e-03  6.157e-04   7.545 4.77e-14 ***
wtd_mean_ElectronAffinity      4.448e-01  4.037e-02  11.018  < 2e-16 ***
gmean_ElectronAffinity         9.764e-02  1.697e-02   5.753 8.94e-09 ***
wtd_gmean_ElectronAffinity    -4.961e-01  3.904e-02 -12.709  < 2e-16 ***
wtd_entropy_ElectronAffinity  -2.312e+01  2.111e+00 -10.950  < 2e-16 ***
range_ElectronAffinity        -3.758e-01  1.952e-02 -19.256  < 2e-16 ***
wtd_range_ElectronAffinity    -1.516e-01  2.071e-02  -7.317 2.66e-13 ***
std_ElectronAffinity           1.168e+00  5.505e-02  21.208  < 2e-16 ***
wtd_std_ElectronAffinity      -4.874e-01  3.711e-02 -13.133  < 2e-16 ***
mean_FusionHeat                1.126e+00  1.466e-01   7.683 1.65e-14 ***
wtd_mean_FusionHeat           -1.252e+00  1.292e-01  -9.692  < 2e-16 ***
gmean_FusionHeat              -9.149e-01  1.374e-01  -6.659 2.85e-11 ***
wtd_gmean_FusionHeat           8.799e-01  1.137e-01   7.739 1.07e-14 ***
entropy_FusionHeat            -1.210e+01  2.917e+00  -4.147 3.38e-05 ***
wtd_entropy_FusionHeat         2.320e+01  2.014e+00  11.517  < 2e-16 ***
range_FusionHeat              -3.247e-01  3.268e-02  -9.937  < 2e-16 ***
wtd_range_FusionHeat           6.318e-01  6.687e-02   9.448  < 2e-16 ***
wtd_mean_ThermalConductivity   4.849e-01  1.978e-02  24.508  < 2e-16 ***
gmean_ThermalConductivity     -9.976e-02  1.551e-02  -6.431 1.30e-10 ***
wtd_gmean_ThermalConductivity -2.980e-01  1.732e-02 -17.206  < 2e-16 ***
entropy_ThermalConductivity    9.472e+00  1.403e+00   6.749 1.55e-11 ***
range_ThermalConductivity     -1.005e-01  1.469e-02  -6.842 8.13e-12 ***
wtd_range_ThermalConductivity -2.217e-01  1.517e-02 -14.618  < 2e-16 ***
std_ThermalConductivity        2.641e-01  3.401e-02   7.766 8.65e-15 ***
gmean_Valence                  6.077e+00  8.847e-01   6.869 6.72e-12 ***
wtd_gmean_Valence             -6.614e+00  8.039e-01  -8.227  < 2e-16 ***
entropy_Valence                8.207e+01  1.077e+01   7.621 2.67e-14 ***
wtd_entropy_Valence           -7.327e+01  4.307e+00 -17.012  < 2e-16 ***
range_Valence                  6.481e+00  4.800e-01  13.504  < 2e-16 ***
wtd_std_Valence               -2.133e+01  1.021e+00 -20.905  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.64 on 14823 degrees of freedom
Multiple R-squared:  0.7358,Adjusted R-squared:  0.7347
F-statistic:   688 on 60 and 14823 DF,  p-value: < 2.2e-16
```

[76]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.reg.b.bic.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 60 predictors is been used"
```

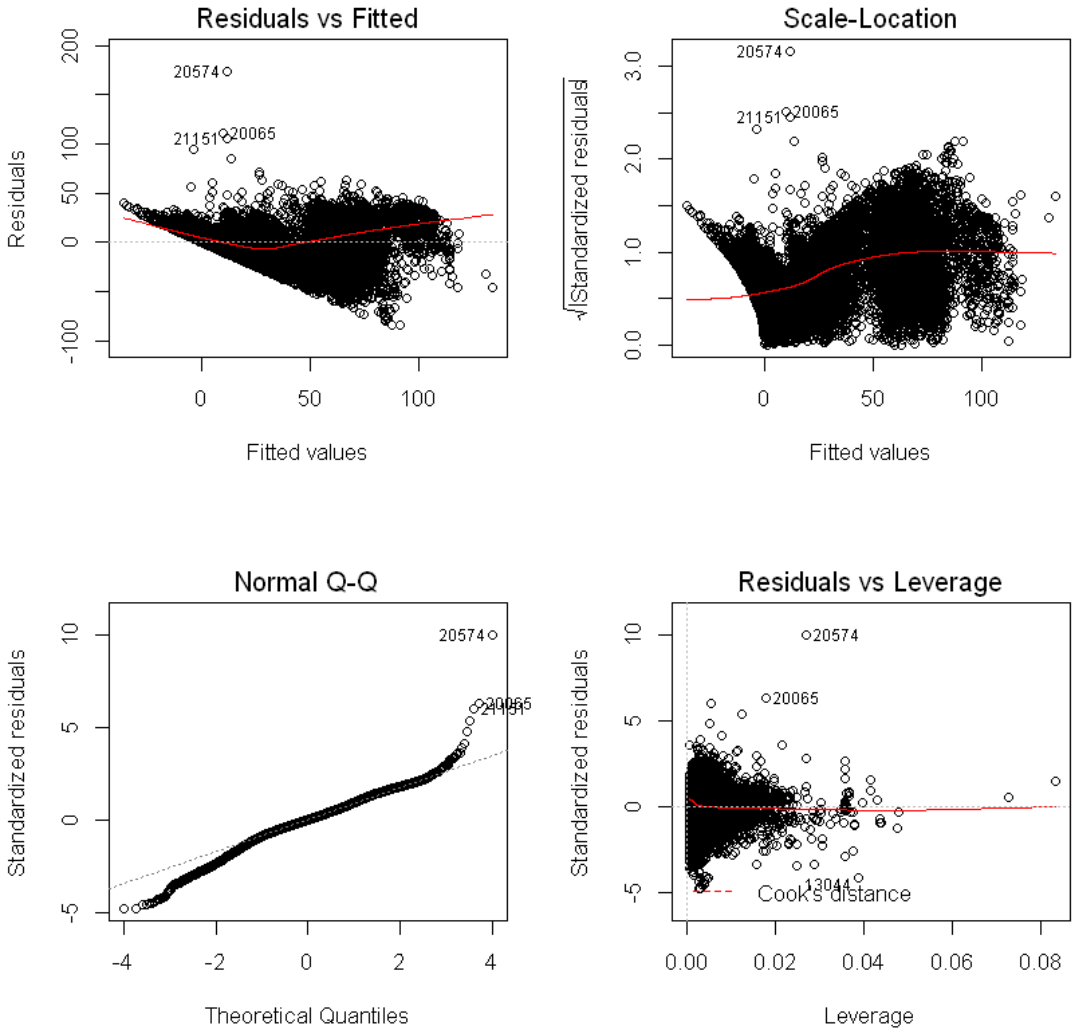
[77]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.all.summary$adj.r.
 ↪squared,4)))
print(paste("Based on Min BIC Val - Adjusted R-Square:",round(fit.reg.b.bic.
 ↪summary$adj.r.squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7355"
[1] "Based on Min BIC Val - Adjusted R-Square: 0.7347"
```

Here we can see that the adjusted R-square is decreased but only for a small amount which indicates that it might be a better model compared to original model(including all predicates) as this model is comparitively less complex

Lets Check the various Residuals plot

[78]:
```
par(mfcol=c(2,2))
plot(fit.reg.b.bic)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if

residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.14 Perform F-tests by comparing the two models using the anova() function

[79]:
```
anova(fit.all, fit.reg.b.bic)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14823	4614922	-21	-20023.8	3.07165	2.690422e-06

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are more correlated as p value is less than 0.05. we can also see that in the new fit the no of predictors is less compared to the original which makes it less complex. Also we can see that there is only slight increase in RSS compared to the original fit. So due to all these factors the new model looks better than the all predictors model

based on Adjusted R Square

So lets start from analysing the best model based on Adjusted R Square ie 76 predictors

[80]:
```
bAdjRSelectedColumns = names(coef(fit.reg.backward,76))
# Chang in the value of '(Intercept) to critical_temp
bAdjRSelectedColumns[1] = 'critical_temp'
bAdjRSelectedColumns
```

1. 'critical_temp' 2. 'number_of_elements' 3. 'mean_atomic_mass' 4. 'wtd_mean_atomic_mass' 5. 'gmean_atomic_mass' 6. 'wtd_gmean_atomic_mass' 7. 'entropy_atomic_mass' 8. 'wtd_entropy_atomic_mass' 9. 'range_atomic_mass' 10. 'wtd_range_atomic_mass' 11. 'std_atomic_mass' 12. 'wtd_std_atomic_mass' 13. 'mean_fie' 14. 'wtd_mean_fie' 15. 'gmean_fie' 16. 'wtd_gmean_fie' 17. 'entropy_fie' 18. 'wtd_entropy_fie' 19. 'range_fie' 20. 'wtd_range_fie' 21. 'std_fie' 22. 'mean_atomic_radius' 23. 'wtd_mean_atomic_radius' 24. 'wtd_gmean_atomic_radius' 25. 'entropy_atomic_radius' 26. 'wtd_entropy_atomic_radius' 27. 'range_atomic_radius' 28. 'wtd_range_atomic_radius' 29. 'std_atomic_radius' 30. 'wtd_std_atomic_radius' 31. 'mean_Density' 32. 'gmean_Density' 33. 'wtd_gmean_Density' 34. 'entropy_Density' 35. 'wtd_entropy_Density' 36. 'range_Density' 37. 'std_Density'

38. 'wtd_std_Density' 39. 'mean_ElectronAffinity' 40. 'wtd_mean_ElectronAffinity' 41. 'gmean_ElectronAffinity' 42. 'wtd_gmean_ElectronAffinity' 43. 'entropy_ElectronAffinity' 44. 'wtd_entropy_ElectronAffinity' 45. 'range_ElectronAffinity' 46. 'wtd_range_ElectronAffinity' 47. 'std_ElectronAffinity' 48. 'wtd_std_ElectronAffinity' 49. 'mean_FusionHeat' 50. 'wtd_mean_FusionHeat' 51. 'gmean_FusionHeat' 52. 'wtd_gmean_FusionHeat' 53. 'entropy_FusionHeat' 54. 'wtd_entropy_FusionHeat' 55. 'range_FusionHeat' 56. 'wtd_range_FusionHeat' 57. 'std_FusionHeat' 58. 'wtd_std_FusionHeat' 59. 'mean_ThermalConductivity' 60. 'wtd_mean_ThermalConductivity' 61. 'gmean_ThermalConductivity' 62. 'wtd_gmean_ThermalConductivity' 63. 'entropy_ThermalConductivity' 64. 'wtd_entropy_ThermalConductivity' 65. 'range_ThermalConductivity' 66. 'wtd_range_ThermalConductivity' 67. 'std_ThermalConductivity' 68. 'mean_Valence' 69. 'wtd_mean_Valence' 70. 'gmean_Valence' 71. 'wtd_gmean_Valence' 72. 'entropy_Valence' 73. 'wtd_entropy_Valence' 74. 'range_Valence' 75. 'wtd_range_Valence' 76. 'std_Valence' 77. 'wtd_std_Valence'

[81]:
```
bAdjRTrain = train[,bAdjRSelectedColumns]
head(bAdjRTrain)
```

	critical_temp	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atc
18847	24.0	6	60.60051	71.50999	46.72851
18895	15.5	4	57.44445	60.35930	56.06791
2986	45.3	6	84.71115	78.84015	66.61372
1842	94.0	7	112.95469	60.86673	82.42970
3371	74.1	6	78.67813	59.21927	58.87964
11638	12.9	3	49.59452	37.84410	37.11177

[82]:
```
fit.reg.b.adjr = lm(critical_temp~., data = bAdjRTrain)
fit.reg.b.adjr.summary = summary(fit.reg.b.adjr)
fit.reg.b.adjr.summary
```

```
Call:
lm(formula = critical_temp ~ ., data = bAdjRTrain)

Residuals:
    Min      1Q  Median      3Q     Max
-84.889  -9.390   0.563  10.906 169.736

Coefficients:
                             Estimate Std. Error t value Pr(>|t|)
(Intercept)                -2.294e+01  5.865e+00  -3.912 9.19e-05 ***
number_of_elements         -3.171e+00  8.786e-01  -3.610 0.000308 ***
mean_atomic_mass            8.101e-01  9.382e-02   8.634  < 2e-16 ***
wtd_mean_atomic_mass       -8.299e-01  1.139e-01  -7.285 3.38e-13 ***
gmean_atomic_mass          -4.383e-01  9.451e-02  -4.638 3.55e-06 ***
wtd_gmean_atomic_mass       5.424e-01  1.100e-01   4.930 8.33e-07 ***
entropy_atomic_mass        -3.890e+01  5.424e+00  -7.171 7.77e-13 ***
wtd_entropy_atomic_mass     7.056e+00  4.161e+00   1.696 0.089938 .
range_atomic_mass           2.173e-01  1.977e-02  10.990  < 2e-16 ***
wtd_range_atomic_mass       3.702e-02  1.996e-02   1.855 0.063634 .
std_atomic_mass            -5.831e-01  7.434e-02  -7.844 4.67e-15 ***
```

```
wtd_std_atomic_mass              9.440e-02  6.241e-02   1.512 0.130436
mean_fie                         2.298e-01  5.233e-02   4.392 1.13e-05 ***
wtd_mean_fie                    -2.887e-01  4.306e-02  -6.706 2.08e-11 ***
gmean_fie                       -2.258e-01  5.160e-02  -4.377 1.21e-05 ***
wtd_gmean_fie                    3.140e-01  4.345e-02   7.228 5.15e-13 ***
entropy_fie                     -1.307e+02  2.309e+01  -5.661 1.53e-08 ***
wtd_entropy_fie                  4.634e+01  5.530e+00   8.380  < 2e-16 ***
range_fie                        6.736e-02  7.770e-03   8.670  < 2e-16 ***
wtd_range_fie                    2.381e-02  4.283e-03   5.560 2.75e-08 ***
std_fie                         -2.140e-01  1.965e-02 -10.890  < 2e-16 ***
mean_atomic_radius              -3.422e-01  3.481e-02  -9.829  < 2e-16 ***
wtd_mean_atomic_radius           2.974e+00  1.884e-01  15.783  < 2e-16 ***
wtd_gmean_atomic_radius         -2.567e+00  1.767e-01 -14.530  < 2e-16 ***
entropy_atomic_radius            8.624e+01  2.060e+01   4.186 2.86e-05 ***
wtd_entropy_atomic_radius        3.800e+01  6.156e+00   6.174 6.83e-10 ***
range_atomic_radius              2.126e-01  2.623e-02   8.106 5.63e-16 ***
wtd_range_atomic_radius         -9.889e-02  1.894e-02  -5.222 1.79e-07 ***
std_atomic_radius               -4.819e-01  8.513e-02  -5.660 1.54e-08 ***
wtd_std_atomic_radius           -2.163e-01  7.442e-02  -2.906 0.003664 **
mean_Density                    -5.079e-03  4.192e-04 -12.115  < 2e-16 ***
gmean_Density                    1.264e-03  4.246e-04   2.975 0.002930 **
wtd_gmean_Density                2.290e-03  3.154e-04   7.261 4.03e-13 ***
entropy_Density                  1.626e+01  3.969e+00   4.098 4.20e-05 ***
wtd_entropy_Density             -1.974e+01  2.836e+00  -6.960 3.55e-12 ***
range_Density                   -1.755e-03  2.564e-04  -6.846 7.88e-12 ***
std_Density                      6.712e-03  7.921e-04   8.473  < 2e-16 ***
wtd_std_Density                 -1.829e-03  5.062e-04  -3.613 0.000304 ***
mean_ElectronAffinity           -7.708e-02  5.537e-02  -1.392 0.163936
wtd_mean_ElectronAffinity        4.959e-01  5.964e-02   8.315  < 2e-16 ***
gmean_ElectronAffinity           1.405e-01  4.800e-02   2.928 0.003417 **
wtd_gmean_ElectronAffinity      -5.361e-01  5.234e-02 -10.242  < 2e-16 ***
entropy_ElectronAffinity         5.649e+00  3.087e+00   1.830 0.067307 .
wtd_entropy_ElectronAffinity    -2.458e+01  2.611e+00  -9.415  < 2e-16 ***
range_ElectronAffinity          -3.788e-01  2.070e-02 -18.300  < 2e-16 ***
wtd_range_ElectronAffinity      -1.612e-01  2.488e-02  -6.478 9.57e-11 ***
std_ElectronAffinity             1.250e+00  6.959e-02  17.959  < 2e-16 ***
wtd_std_ElectronAffinity        -5.287e-01  4.543e-02 -11.637  < 2e-16 ***
mean_FusionHeat                  1.635e+00  2.214e-01   7.385 1.61e-13 ***
wtd_mean_FusionHeat             -1.892e+00  2.227e-01  -8.496  < 2e-16 ***
gmean_FusionHeat                -1.406e+00  2.017e-01  -6.968 3.36e-12 ***
wtd_gmean_FusionHeat             1.493e+00  2.053e-01   7.273 3.69e-13 ***
entropy_FusionHeat              -1.805e+01  3.256e+00  -5.543 3.02e-08 ***
wtd_entropy_FusionHeat           2.552e+01  2.284e+00  11.174  < 2e-16 ***
range_FusionHeat                -3.736e-01  7.921e-02  -4.716 2.42e-06 ***
wtd_range_FusionHeat             6.604e-01  7.962e-02   8.295  < 2e-16 ***
std_FusionHeat                  -4.401e-01  3.076e-01  -1.431 0.152488
wtd_std_FusionHeat               6.302e-01  1.793e-01   3.516 0.000440 ***
mean_ThermalConductivity        -4.329e-02  2.680e-02  -1.616 0.106197
```

```
wtd_mean_ThermalConductivity     5.068e-01  2.442e-02  20.755  < 2e-16 ***
gmean_ThermalConductivity       -7.876e-02  2.310e-02  -3.410 0.000652 ***
wtd_gmean_ThermalConductivity   -3.109e-01  1.949e-02 -15.951  < 2e-16 ***
entropy_ThermalConductivity      9.925e+00  2.268e+00   4.375 1.22e-05 ***
wtd_entropy_ThermalConductivity  2.998e+00  1.716e+00   1.747 0.080591 .
range_ThermalConductivity       -9.614e-02  1.575e-02  -6.104 1.06e-09 ***
wtd_range_ThermalConductivity   -2.211e-01  1.905e-02 -11.606  < 2e-16 ***
std_ThermalConductivity          2.828e-01  4.479e-02   6.314 2.79e-10 ***
mean_Valence                    -1.741e+01  7.204e+00  -2.417 0.015677 *
wtd_mean_Valence                 2.890e+01  8.599e+00   3.361 0.000779 ***
gmean_Valence                    2.143e+01  6.806e+00   3.149 0.001642 **
wtd_gmean_Valence               -3.279e+01  8.081e+00  -4.057 4.99e-05 ***
entropy_Valence                  8.006e+01  1.440e+01   5.560 2.74e-08 ***
wtd_entropy_Valence             -6.629e+01  6.385e+00 -10.383  < 2e-16 ***
range_Valence                    5.714e+00  8.784e-01   6.505 8.03e-11 ***
wtd_range_Valence               -9.006e-01  7.288e-01  -1.236 0.216605
std_Valence                      6.170e+00  2.917e+00   2.115 0.034430 *
wtd_std_Valence                 -2.720e+01  2.258e+00 -12.045  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.62 on 14807 degrees of freedom
Multiple R-squared:  0.7369,Adjusted R-squared:  0.7356
F-statistic: 545.7 on 76 and 14807 DF,  p-value: < 2.2e-16
```

[83]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.reg.b.adjr.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 76 predictors is been used"
```

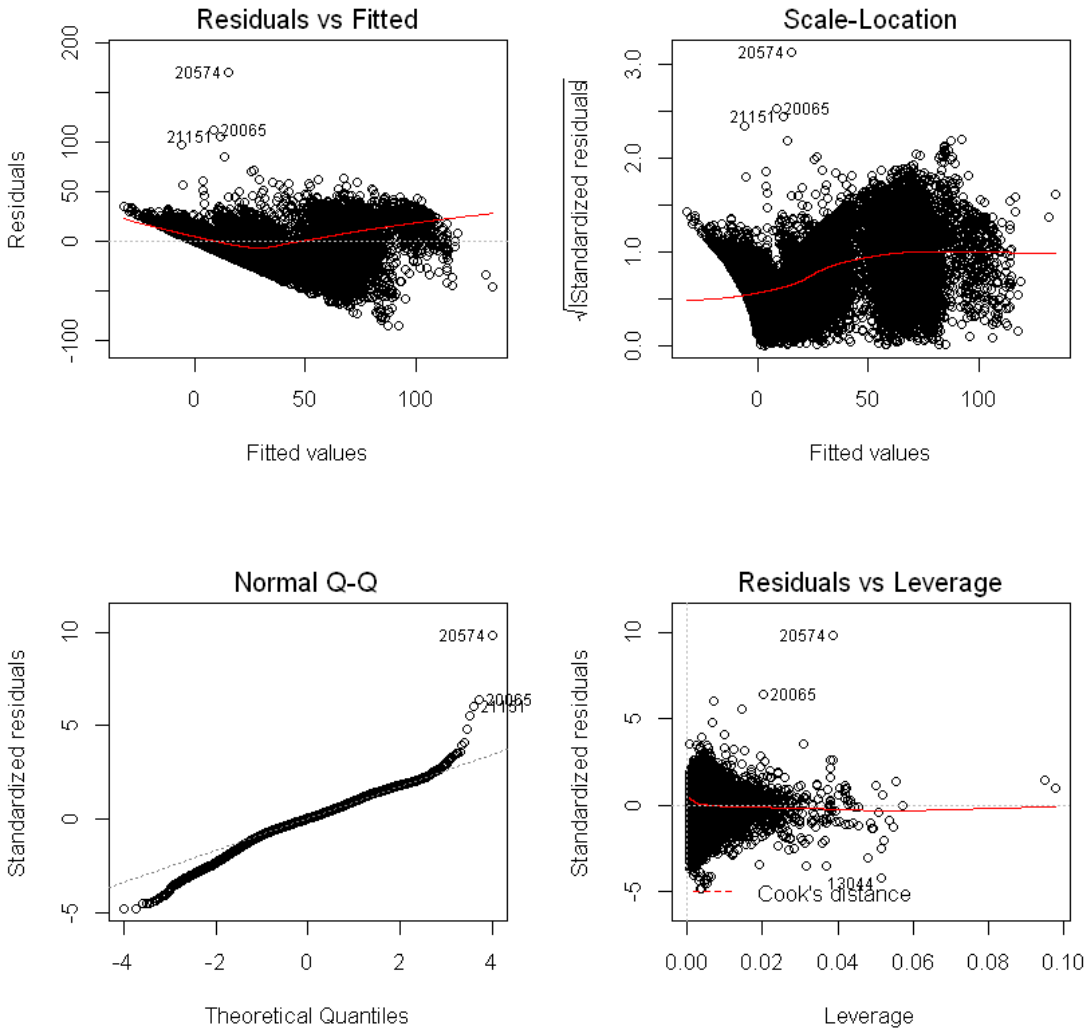
[84]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.all.summary$adj.r.
 ↪squared,4)))
print(paste("Backward Subset Selection Max Adjusted R Square Val - Adjusted␣
 ↪R-Square:",round(fit.reg.b.adjr.summary$adj.r.squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7355"
[1] "Backward Subset Selection Max Adjusted R Square Val - Adjusted R-Square:
0.7356"
```

Here we can see that the adjusted R-square is increased which indicates that it might be a better model compared to original model(including all predicates) as this model is comparitively less complex

Lets Check the various Residuals plot

[85]:
```
par(mfcol=c(2,2))
plot(fit.reg.b.adjr)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For

example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.15 Perform F-tests by comparing the two models using the anova() function

[86]:
```
anova(fit.all, fit.reg.b.adjr)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14807	4595301	-5	-402.2139	0.2591383	0.9353668

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are not much correlated as p value is greater than 0.05. we can also see that in the new fit the no of predictors is less compared to the original which makes it less complex. Also we can see that there is only slight increase in RSS compared to the original fit. So due to all these factors the new model looks better than the all predictors model

based on Cp

[87]:
```
bCpSelectedColumns = names(coef(fit.reg.backward,70))
# Changing in the value of '(Intercept) to critical_temp
bCpSelectedColumns[1] = 'critical_temp'
bCpSelectedColumns
```

1. 'critical_temp' 2. 'number_of_elements' 3. 'mean_atomic_mass' 4. 'wtd_mean_atomic_mass' 5. 'gmean_atomic_mass' 6. 'wtd_gmean_atomic_mass' 7. 'entropy_atomic_mass' 8. 'range_atomic_mass' 9. 'std_atomic_mass' 10. 'mean_fie' 11. 'wtd_mean_fie' 12. 'gmean_fie' 13. 'wtd_gmean_fie' 14. 'entropy_fie' 15. 'wtd_entropy_fie' 16. 'range_fie' 17. 'wtd_range_fie' 18. 'std_fie' 19. 'mean_atomic_radius' 20. 'wtd_mean_atomic_radius' 21. 'wtd_gmean_atomic_radius' 22. 'entropy_atomic_radius' 23. 'wtd_entropy_atomic_radius' 24. 'range_atomic_radius' 25. 'wtd_range_atomic_radius'

26. 'std_atomic_radius' 27. 'wtd_std_atomic_radius' 28. 'mean_Density' 29. 'gmean_Density' 30. 'wtd_gmean_Density' 31. 'entropy_Density' 32. 'wtd_entropy_Density' 33. 'range_Density' 34. 'std_Density' 35. 'wtd_std_Density' 36. 'wtd_mean_ElectronAffinity' 37. 'gmean_ElectronAffinity' 38. 'wtd_gmean_ElectronAffinity' 39. 'entropy_ElectronAffinity' 40. 'wtd_entropy_ElectronAffinity' 41. 'range_ElectronAffinity' 42. 'wtd_range_ElectronAffinity' 43. 'std_ElectronAffinity' 44. 'wtd_std_ElectronAffinity' 45. 'mean_FusionHeat' 46. 'wtd_mean_FusionHeat' 47. 'gmean_FusionHeat' 48. 'wtd_gmean_FusionHeat' 49. 'entropy_FusionHeat' 50. 'wtd_entropy_FusionHeat' 51. 'range_FusionHeat' 52. 'wtd_range_FusionHeat' 53. 'wtd_std_FusionHeat' 54. 'mean_ThermalConductivity' 55. 'wtd_mean_ThermalConductivity' 56. 'gmean_ThermalConductivity' 57. 'wtd_gmean_ThermalConductivity' 58. 'entropy_ThermalConductivity' 59. 'wtd_entropy_ThermalConductivity' 60. 'range_ThermalConductivity' 61. 'wtd_range_ThermalConductivity' 62. 'std_ThermalConductivity' 63. 'mean_Valence' 64. 'wtd_mean_Valence' 65. 'gmean_Valence' 66. 'wtd_gmean_Valence' 67. 'entropy_Valence' 68. 'wtd_entropy_Valence' 69. 'range_Valence' 70. 'std_Valence' 71. 'wtd_std_Valence'

[88]:
```
bCpTrain = train[,bCpSelectedColumns]
head(bCpTrain)
```

	critical_temp	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atc
18847	24.0	6	60.60051	71.50999	46.72851
18895	15.5	4	57.44445	60.35930	56.06791
2986	45.3	6	84.71115	78.84015	66.61372
1842	94.0	7	112.95469	60.86673	82.42970
3371	74.1	6	78.67813	59.21927	58.87964
11638	12.9	3	49.59452	37.84410	37.11177

[89]:
```
fit.reg.b.cp = lm(critical_temp~., data = bCpTrain)
fit.reg.b.cp.summary = summary(fit.reg.b.cp)
fit.reg.b.cp.summary
```

```
Call:
lm(formula = critical_temp ~ ., data = bCpTrain)

Residuals:
    Min      1Q  Median      3Q     Max
-84.670  -9.424   0.544  10.953 169.681

Coefficients:
                            Estimate Std. Error t value Pr(>|t|)
(Intercept)               -2.255e+01  5.810e+00  -3.881 0.000104 ***
number_of_elements        -3.138e+00  8.643e-01  -3.631 0.000284 ***
mean_atomic_mass           7.706e-01  7.192e-02  10.715  < 2e-16 ***
wtd_mean_atomic_mass      -7.381e-01  6.231e-02 -11.844  < 2e-16 ***
gmean_atomic_mass         -4.124e-01  7.647e-02  -5.394 7.01e-08 ***
wtd_gmean_atomic_mass      4.761e-01  6.676e-02   7.131 1.04e-12 ***
entropy_atomic_mass       -3.370e+01  4.893e+00  -6.888 5.89e-12 ***
range_atomic_mass          2.137e-01  1.963e-02  10.889  < 2e-16 ***
std_atomic_mass           -4.915e-01  5.304e-02  -9.267  < 2e-16 ***
mean_fie                   2.297e-01  5.201e-02   4.416 1.01e-05 ***
```

```
wtd_mean_fie                    -2.897e-01  4.236e-02  -6.839 8.30e-12 ***
gmean_fie                       -2.281e-01  5.124e-02  -4.452 8.56e-06 ***
wtd_gmean_fie                    3.169e-01  4.253e-02   7.452 9.72e-14 ***
entropy_fie                     -1.268e+02  2.292e+01  -5.533 3.19e-08 ***
wtd_entropy_fie                  4.458e+01  5.255e+00   8.483  < 2e-16 ***
range_fie                        6.943e-02  7.676e-03   9.046  < 2e-16 ***
wtd_range_fie                    2.327e-02  3.865e-03   6.022 1.76e-09 ***
std_fie                         -2.183e-01  1.954e-02 -11.169  < 2e-16 ***
mean_atomic_radius              -3.348e-01  3.322e-02 -10.078  < 2e-16 ***
wtd_mean_atomic_radius           2.936e+00  1.827e-01  16.068  < 2e-16 ***
wtd_gmean_atomic_radius         -2.541e+00  1.723e-01 -14.746  < 2e-16 ***
entropy_atomic_radius            7.396e+01  2.018e+01   3.665 0.000248 ***
wtd_entropy_atomic_radius        4.364e+01  4.688e+00   9.308  < 2e-16 ***
range_atomic_radius              2.096e-01  2.605e-02   8.045 9.29e-16 ***
wtd_range_atomic_radius         -9.162e-02  1.463e-02  -6.265 3.84e-10 ***
std_atomic_radius               -5.035e-01  8.471e-02  -5.943 2.86e-09 ***
wtd_std_atomic_radius           -1.922e-01  7.354e-02  -2.613 0.008984 **
mean_Density                    -5.046e-03  4.153e-04 -12.151  < 2e-16 ***
gmean_Density                    1.231e-03  4.214e-04   2.923 0.003475 **
wtd_gmean_Density                2.315e-03  3.114e-04   7.432 1.13e-13 ***
entropy_Density                  1.460e+01  3.838e+00   3.803 0.000143 ***
wtd_entropy_Density             -1.744e+01  2.458e+00  -7.094 1.36e-12 ***
range_Density                   -1.761e-03  2.534e-04  -6.949 3.82e-12 ***
std_Density                      6.392e-03  7.734e-04   8.264  < 2e-16 ***
wtd_std_Density                 -1.466e-03  4.567e-04  -3.209 0.001333 **
wtd_mean_ElectronAffinity        4.402e-01  4.156e-02  10.590  < 2e-16 ***
gmean_ElectronAffinity           8.096e-02  2.059e-02   3.931 8.49e-05 ***
wtd_gmean_ElectronAffinity      -4.925e-01  3.998e-02 -12.318  < 2e-16 ***
entropy_ElectronAffinity         5.481e+00  3.065e+00   1.788 0.073760 .
wtd_entropy_ElectronAffinity    -2.467e+01  2.557e+00  -9.651  < 2e-16 ***
range_ElectronAffinity          -3.805e-01  2.055e-02 -18.520  < 2e-16 ***
wtd_range_ElectronAffinity      -1.620e-01  2.329e-02  -6.954 3.69e-12 ***
std_ElectronAffinity             1.205e+00  6.334e-02  19.022  < 2e-16 ***
wtd_std_ElectronAffinity        -4.900e-01  3.848e-02 -12.734  < 2e-16 ***
mean_FusionHeat                  1.447e+00  1.656e-01   8.739  < 2e-16 ***
wtd_mean_FusionHeat             -1.683e+00  1.834e-01  -9.176  < 2e-16 ***
gmean_FusionHeat                -1.256e+00  1.622e-01  -7.741 1.05e-14 ***
wtd_gmean_FusionHeat             1.328e+00  1.792e-01   7.411 1.32e-13 ***
entropy_FusionHeat              -1.713e+01  3.047e+00  -5.624 1.90e-08 ***
wtd_entropy_FusionHeat           2.371e+01  2.069e+00  11.462  < 2e-16 ***
range_FusionHeat                -4.738e-01  4.754e-02  -9.966  < 2e-16 ***
wtd_range_FusionHeat             5.976e-01  6.774e-02   8.821  < 2e-16 ***
wtd_std_FusionHeat               4.295e-01  1.274e-01   3.371 0.000752 ***
mean_ThermalConductivity        -5.450e-02  2.627e-02  -2.075 0.038033 *
wtd_mean_ThermalConductivity     5.137e-01  2.402e-02  21.384  < 2e-16 ***
gmean_ThermalConductivity       -7.516e-02  2.276e-02  -3.302 0.000962 ***
wtd_gmean_ThermalConductivity   -3.105e-01  1.934e-02 -16.055  < 2e-16 ***
entropy_ThermalConductivity      1.062e+01  2.245e+00   4.731 2.26e-06 ***
```

```
wtd_entropy_ThermalConductivity  2.873e+00  1.685e+00   1.705 0.088274 .
range_ThermalConductivity       -9.749e-02  1.571e-02  -6.206 5.58e-10 ***
wtd_range_ThermalConductivity   -2.231e-01  1.877e-02 -11.891  < 2e-16 ***
std_ThermalConductivity          2.912e-01  4.458e-02   6.531 6.73e-11 ***
mean_Valence                    -1.532e+01  6.901e+00  -2.219 0.026486 *
wtd_mean_Valence                 2.665e+01  7.989e+00   3.336 0.000853 ***
gmean_Valence                    1.966e+01  6.563e+00   2.995 0.002749 **
wtd_gmean_Valence               -3.119e+01  7.580e+00  -4.114 3.91e-05 ***
entropy_Valence                  8.363e+01  1.412e+01   5.923 3.22e-09 ***
wtd_entropy_Valence             -6.315e+01  5.702e+00 -11.075  < 2e-16 ***
range_Valence                    5.845e+00  8.707e-01   6.713 1.97e-11 ***
std_Valence                      5.630e+00  2.798e+00   2.012 0.044238 *
wtd_std_Valence                 -2.699e+01  2.116e+00 -12.753  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.62 on 14813 degrees of freedom
Multiple R-squared:  0.7367,Adjusted R-squared:  0.7355
F-statistic: 592.2 on 70 and 14813 DF,  p-value: < 2.2e-16
```

[90]:
```
# -1 to remove the row with value as intercept
print(paste("we can see that in this model around", nrow(fit.reg.b.cp.
 ↪summary$coefficients)-1,"predictors is been used"))
```

```
[1] "we can see that in this model around 70 predictors is been used"
```

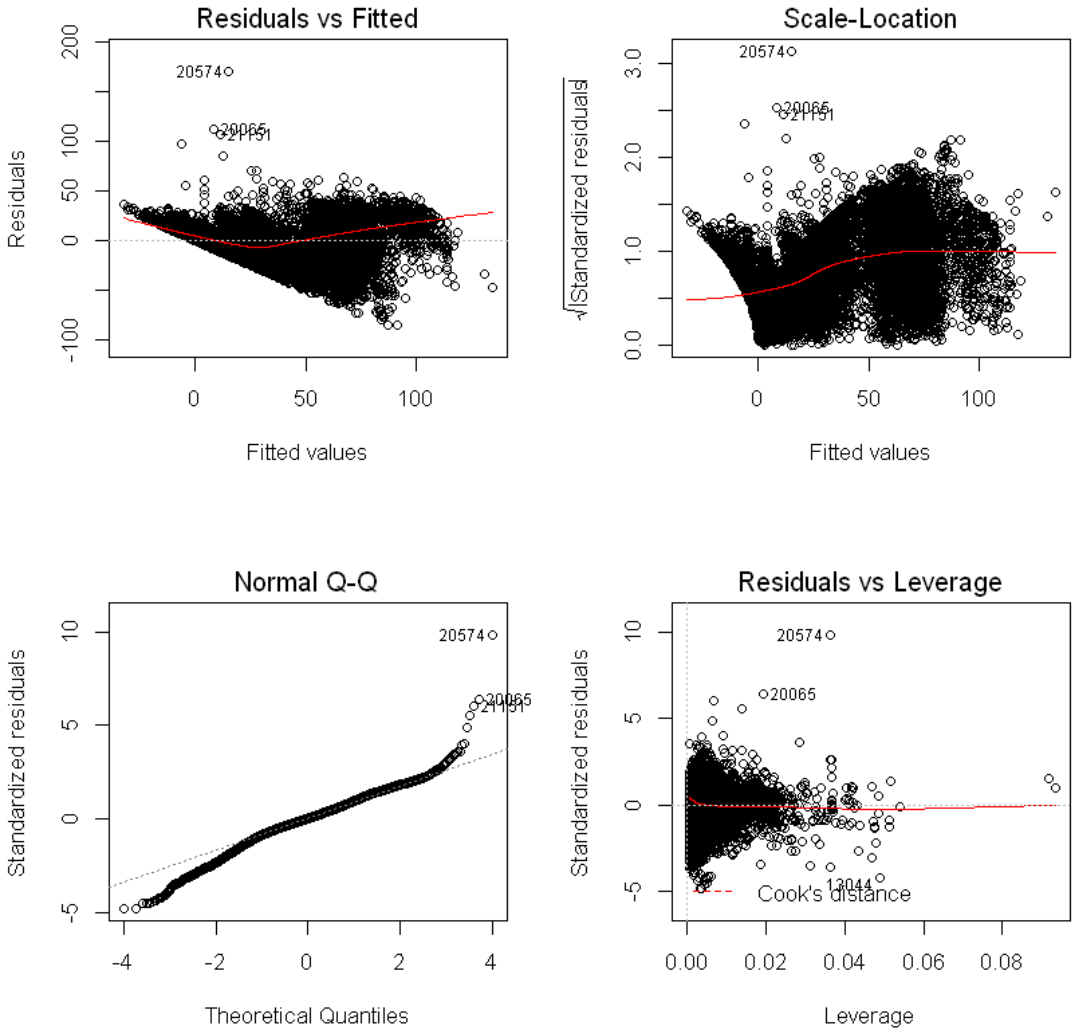
[91]:
```
print(paste("All Predictors - Adjusted R-Square:",round(fit.all.summary$adj.r.
 ↪squared,4)))
print(paste("Based on Min Cp Val - Adjusted R-Square:",round(fit.reg.b.cp.
 ↪summary$adj.r.squared,4)))
```

```
[1] "All Predictors - Adjusted R-Square: 0.7355"
[1] "Based on Min Cp Val - Adjusted R-Square: 0.7355"
```

Here we can see that the adjusted R-square is decreased but only for a small amount which indicates that it might be a better model compared to original model(including all predicates) as this model is comparitively less complex

Lets Check the various Residuals plot

[92]:
```
par(mfcol=c(2,2))
plot(fit.reg.b.cp)
```



Analysis on the four plots

The **residual vs fitted plot**: This plot is used to check the linear assumption. It shows if residuals have non-linear patterns. If you find equally spread residuals around a horizontal line without distinct patterns, that is a good indication you have linear relationships. However, if the relationship between predictors and an response variable is non-linear, an obvious pattern could show up in this plot if the model cannot capture the non-linearity. The first plot above shows that there could be a non-linear relationship between critical_temp and all the predictors, as the residuals are not scattered evenly.

The normal **Q-Q plot**: The Q-Q plot (i.e., quantile-quantile plot) is a graphical tool to help us assess if a set of data plausibly came from some theoretical distribution such as a Normal. For example, if we run a statistical analysis that assumes our dependent variable is Normally distributed, we can use a Normal Q-Q plot to check that assumption. In the case of linear regression analysis, we assume that residual is normally distributed with constant variance and mean equal to zero. The normal Q-Q plot shows if residuals are normally distributed. Generally It is good if

residuals are lined well on the straight dashed line. In the above Plot it seems that the residuals are approximatly distributed normally

The **scale-location plot**: It is used to check the assumption of equal variance by showing if residuals are spread equally along the ranges of predictors. It is good if we can see a horizontal line with equally (randomly) spread points. The scale-location plot shows that the residuals appear randomly spread.

The **residual-leverage plot**: it helps us identify influential data samples. Not all outliers are influential in linear regression analysis. Here we care about the samples that are influential to determine the regression line. These samples can very influential even if they look to be within a reasonable range of the values. They can alter the results if we exclude them from analysis. In the residual-leverage plot, we look for outlying values at the upper right corner or at the lower right corner. Samples located in those places can be influential against a regression line. We usually use Cook's distance, indicated by a red dash line. When samples are outside of the Cook's distance (i.e, they have high Cook's distance scores, Cook's distance measures how much the entire regression function changes when the i-th case is deleted.), the samples are influential to the regression results. The regression results will be altered if we exclude those samples. Here in this plot we can barely see Cook's distance lines because all cases are well inside of the Cook's distance lines. Therefore no influential cases are observed.

4.1.16 Perform F-tests by comparing the two models using the anova() function

[93]:
```
anova(fit.all, fit.reg.b.cp)
```

Res.Df	RSS	Df	Sum of Sq	F	Pr(>F)
14802	4594899	NA	NA	NA	NA
14813	4598388	-11	-3488.991	1.021766	0.4234977

Here with respect to the original Fit (including all predicators) we can see that in the new model the predictors are not much correlated as p value is greater than 0.05. we can also see that in the new fit the no of predictors is less compared to the original which makes it less complex. Also we can see that there is only slight increase in RSS compared to the original fit. So due to all these factors the new model looks better than the all predictors model

5 Model Accuracy Analysis

5.1 Mean Square Error

[94]:
```
print(paste("allPredictorsFit --",mean((predict(fit.all, test, type="response")␣
 ↪- test$critical_temp)^2)))
print(paste("highlyCorrelatedTrain --",mean((predict(fit.correlated, test,␣
 ↪type="response") - test$critical_temp)^2)))
print(paste("Backward Subset Selection(Min BIC) --",mean((predict(fit.reg.b.
 ↪bic, test, type="response") - test$critical_temp)^2)))
print(paste("Backward Subset Selection(Max Adjusted R Square)␣
 ↪--",mean((predict(fit.reg.b.adjr, test, type="response") -␣
 ↪test$critical_temp)^2)))
print(paste("Backward Subset Selection(Min Cp) --",mean((predict(fit.reg.b.cp,␣
 ↪test, type="response") - test$critical_temp)^2)))
```

```
print(paste("Forward Subset Selection(Min BIC) --",mean((predict(fit.reg.f.bic,␣
 ↪test, type="response") - test$critical_temp)^2)))
print(paste("allStarredFit --",mean((predict(fit.starred, test,␣
 ↪type="response") - test$critical_temp)^2)))
print(paste("stepBackwardFit --",mean((predict(fit.step.backward, test,␣
 ↪type="response") - test$critical_temp)^2)))
print(paste("stepForwardFit --",mean((predict(fit.step.forward, test,␣
 ↪type="response") - test$critical_temp)^2)))
```

```
[1] "allPredictorsFit -- 308.659073948539"
[1] "highlyCorrelatedTrain -- 407.498966463707"
[1] "Backward Subset Selection(Min BIC) -- 310.038796898743"
[1] "Backward Subset Selection(Max Adjusted R Square) -- 308.692559505932"
[1] "Backward Subset Selection(Min Cp) -- 308.808740104244"
[1] "Forward Subset Selection(Min BIC) -- 308.72306329421"
[1] "allStarredFit -- 309.09531579758"
[1] "stepBackwardFit -- 308.808740104244"
[1] "stepForwardFit -- 308.522895393448"
```

Here except for the highlyCorrelatedTrain all other models have almost same mean square error. So for rest of the models we can also compare its adjusted R square value and also no of predictors used to determine which is the best model.

5.2 Adjusted R Square of Different Models

[95]:
```
print(paste("allPredictorsFit --",round(fit.all.summary$adj.r.squared,4)))
print(paste("Backward Subset Selection(Min BIC) --",round(fit.reg.b.bic.
 ↪summary$adj.r.squared,4)))
print(paste("Backward Subset Selection(Max Adjusted R Square) --",round(fit.reg.
 ↪b.adjr.summary$adj.r.squared,4)))
print(paste("Backward Subset Selection(Min Cp) --",round(fit.reg.b.cp.
 ↪summary$adj.r.squared,4)))
print(paste("Forward Subset Selection(Min BIC) --",round(fit.reg.f.bic.
 ↪summary$adj.r.squared,4)))
print(paste("allStarredFit --",round(fit.starred.summary$adj.r.squared,4)))
print(paste("stepBackwardFit --",round(fit.step.backward.summary$adj.r.
 ↪squared,4)))
print(paste("stepForwardFit --",round(fit.step.forward.summary$adj.r.
 ↪squared,4)))
```

```
[1] "allPredictorsFit -- 0.7355"
[1] "Backward Subset Selection(Min BIC) -- 0.7347"
[1] "Backward Subset Selection(Max Adjusted R Square) -- 0.7356"
[1] "Backward Subset Selection(Min Cp) -- 0.7355"
[1] "Forward Subset Selection(Min BIC) -- 0.7352"
[1] "allStarredFit -- 0.7353"
```

```
[1] "stepBackwardFit -- 0.7355"
[1] "stepForwardFit -- 0.7354"
```

Here we can see that the adjusted R square values are also approximately same for all the models. So lets make a decision based on the no of predictors

5.3 No of Predictors Used

[96]:
```
print(paste("allPredictorsFit --",nrow(fit.all.summary$coefficients)-1))
print(paste("Backward Subset Selection(Min BIC) --",nrow(fit.reg.b.bic.
 ↪summary$coefficients)-1))
print(paste("Backward Subset Selection(Max Adjusted R Square) --",nrow(fit.reg.
 ↪b.adjr.summary$coefficients)-1))
print(paste("Backward Subset Selection(Min Cp) --",nrow(fit.reg.b.cp.
 ↪summary$coefficients)-1))
print(paste("Forward Subset Selection(Min BIC) --",nrow(fit.reg.f.bic.
 ↪summary$coefficients)-1))
print(paste("allStarredFit --",nrow(fit.starred.summary$coefficients)-1))
print(paste("stepBackwardFit --",nrow(fit.step.backward.
 ↪summary$coefficients)-1))
print(paste("stepForwardFit --",nrow(fit.step.forward.summary$coefficients)-1))
```

```
[1] "allPredictorsFit -- 81"
[1] "Backward Subset Selection(Min BIC) -- 60"
[1] "Backward Subset Selection(Max Adjusted R Square) -- 76"
[1] "Backward Subset Selection(Min Cp) -- 70"
[1] "Forward Subset Selection(Min BIC) -- 73"
[1] "allStarredFit -- 67"
[1] "stepBackwardFit -- 70"
[1] "stepForwardFit -- 77"
```

Here we can see that the Model that we selected using backward subset selection and which had the min BIC value can be considered as the best model out of these models as it is more simple model compared to rest of the models. As it is able to almost predict the values with just 60 predictors

Summary of the model that we have selected is shown below

[97]:
```
fit.reg.b.bic.summary
```

```
Call:
lm(formula = critical_temp ~ ., data = bBicTrain)

Residuals:
    Min      1Q  Median      3Q     Max
-84.157  -9.440   0.561  10.958 173.433

Coefficients:
                                Estimate Std. Error t value Pr(>|t|)
```

(Intercept)	-1.899e+01	5.708e+00	-3.327	0.000880	***
number_of_elements	-3.485e+00	8.522e-01	-4.090	4.33e-05	***
mean_atomic_mass	8.318e-01	6.316e-02	13.169	< 2e-16	***
wtd_mean_atomic_mass	-8.596e-01	5.118e-02	-16.795	< 2e-16	***
gmean_atomic_mass	-4.434e-01	6.567e-02	-6.752	1.51e-11	***
wtd_gmean_atomic_mass	5.653e-01	5.627e-02	10.046	< 2e-16	***
entropy_atomic_mass	-3.705e+01	4.712e+00	-7.862	4.03e-15	***
range_atomic_mass	2.138e-01	1.903e-02	11.233	< 2e-16	***
std_atomic_mass	-4.936e-01	5.156e-02	-9.575	< 2e-16	***
mean_fie	2.576e-01	4.801e-02	5.365	8.22e-08	***
wtd_mean_fie	-2.937e-01	3.998e-02	-7.346	2.14e-13	***
gmean_fie	-2.589e-01	4.753e-02	-5.447	5.20e-08	***
wtd_gmean_fie	3.171e-01	4.038e-02	7.854	4.31e-15	***
entropy_fie	-1.032e+02	2.098e+01	-4.918	8.86e-07	***
wtd_entropy_fie	5.068e+01	4.661e+00	10.873	< 2e-16	***
range_fie	7.046e-02	7.443e-03	9.468	< 2e-16	***
wtd_range_fie	2.171e-02	3.760e-03	5.772	7.98e-09	***
std_fie	-2.165e-01	1.911e-02	-11.330	< 2e-16	***
mean_atomic_radius	-3.085e-01	2.928e-02	-10.535	< 2e-16	***
wtd_mean_atomic_radius	2.616e+00	1.195e-01	21.881	< 2e-16	***
wtd_gmean_atomic_radius	-2.243e+00	1.168e-01	-19.206	< 2e-16	***
entropy_atomic_radius	5.822e+01	1.878e+01	3.101	0.001934	**
wtd_entropy_atomic_radius	4.791e+01	4.297e+00	11.150	< 2e-16	***
range_atomic_radius	2.009e-01	2.559e-02	7.852	4.37e-15	***
wtd_range_atomic_radius	-7.278e-02	1.403e-02	-5.189	2.15e-07	***
std_atomic_radius	-6.128e-01	6.690e-02	-9.161	< 2e-16	***
mean_Density	-4.480e-03	3.009e-04	-14.891	< 2e-16	***
wtd_gmean_Density	3.059e-03	2.659e-04	11.506	< 2e-16	***
entropy_Density	1.196e+01	3.521e+00	3.396	0.000684	***
wtd_entropy_Density	-1.550e+01	2.183e+00	-7.102	1.28e-12	***
range_Density	-1.643e-03	2.489e-04	-6.601	4.22e-11	***
std_Density	4.645e-03	6.157e-04	7.545	4.77e-14	***
wtd_mean_ElectronAffinity	4.448e-01	4.037e-02	11.018	< 2e-16	***
gmean_ElectronAffinity	9.764e-02	1.697e-02	5.753	8.94e-09	***
wtd_gmean_ElectronAffinity	-4.961e-01	3.904e-02	-12.709	< 2e-16	***
wtd_entropy_ElectronAffinity	-2.312e+01	2.111e+00	-10.950	< 2e-16	***
range_ElectronAffinity	-3.758e-01	1.952e-02	-19.256	< 2e-16	***
wtd_range_ElectronAffinity	-1.516e-01	2.071e-02	-7.317	2.66e-13	***
std_ElectronAffinity	1.168e+00	5.505e-02	21.208	< 2e-16	***
wtd_std_ElectronAffinity	-4.874e-01	3.711e-02	-13.133	< 2e-16	***
mean_FusionHeat	1.126e+00	1.466e-01	7.683	1.65e-14	***
wtd_mean_FusionHeat	-1.252e+00	1.292e-01	-9.692	< 2e-16	***
gmean_FusionHeat	-9.149e-01	1.374e-01	-6.659	2.85e-11	***
wtd_gmean_FusionHeat	8.799e-01	1.137e-01	7.739	1.07e-14	***
entropy_FusionHeat	-1.210e+01	2.917e+00	-4.147	3.38e-05	***
wtd_entropy_FusionHeat	2.320e+01	2.014e+00	11.517	< 2e-16	***
range_FusionHeat	-3.247e-01	3.268e-02	-9.937	< 2e-16	***
wtd_range_FusionHeat	6.318e-01	6.687e-02	9.448	< 2e-16	***

```
wtd_mean_ThermalConductivity   4.849e-01  1.978e-02  24.508  < 2e-16 ***
gmean_ThermalConductivity     -9.976e-02  1.551e-02  -6.431 1.30e-10 ***
wtd_gmean_ThermalConductivity -2.980e-01  1.732e-02 -17.206  < 2e-16 ***
entropy_ThermalConductivity    9.472e+00  1.403e+00   6.749 1.55e-11 ***
range_ThermalConductivity     -1.005e-01  1.469e-02  -6.842 8.13e-12 ***
wtd_range_ThermalConductivity -2.217e-01  1.517e-02 -14.618  < 2e-16 ***
std_ThermalConductivity        2.641e-01  3.401e-02   7.766 8.65e-15 ***
gmean_Valence                  6.077e+00  8.847e-01   6.869 6.72e-12 ***
wtd_gmean_Valence             -6.614e+00  8.039e-01  -8.227  < 2e-16 ***
entropy_Valence                8.207e+01  1.077e+01   7.621 2.67e-14 ***
wtd_entropy_Valence           -7.327e+01  4.307e+00 -17.012  < 2e-16 ***
range_Valence                  6.481e+00  4.800e-01  13.504  < 2e-16 ***
wtd_std_Valence               -2.133e+01  1.021e+00 -20.905  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 17.64 on 14823 degrees of freedom
Multiple R-squared:  0.7358,Adjusted R-squared:  0.7347
F-statistic:   688 on 60 and 14823 DF,  p-value: < 2.2e-16
```

Based on This The subset of Attributes That act as most significant are:

[110]:
```
coef(fit.reg.b.bic.summary)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	-1.898970e+01	5.707739e+00	-3.327010	8.799685e-04
number_of_elements	-3.485466e+00	8.521721e-01	-4.090097	4.334717e-05
mean_atomic_mass	8.318261e-01	6.316356e-02	13.169398	2.190451e-39
wtd_mean_atomic_mass	-8.595754e-01	5.117994e-02	-16.795163	1.005736e-62
gmean_atomic_mass	-4.434414e-01	6.567111e-02	-6.752458	1.507671e-11
wtd_gmean_atomic_mass	5.652504e-01	5.626547e-02	10.046133	1.137461e-23
entropy_atomic_mass	-3.704529e+01	4.711674e+00	-7.862448	4.025357e-15
range_atomic_mass	2.138135e-01	1.903431e-02	11.233056	3.680340e-29
std_atomic_mass	-4.936423e-01	5.155537e-02	-9.574993	1.176704e-21
mean_fie	2.575825e-01	4.801293e-02	5.364858	8.222986e-08
wtd_mean_fie	-2.937184e-01	3.998217e-02	-7.346236	2.144911e-13
gmean_fie	-2.588955e-01	4.752866e-02	-5.447144	5.200086e-08
wtd_gmean_fie	3.171125e-01	4.037722e-02	7.853748	4.313555e-15
entropy_fie	-1.031519e+02	2.097628e+01	-4.917550	8.857289e-07
wtd_entropy_fie	5.068150e+01	4.661164e+00	10.873142	1.964551e-27
range_fie	7.046231e-02	7.442514e-03	9.467542	3.288893e-21
wtd_range_fie	2.170597e-02	3.760474e-03	5.772136	7.983836e-09
std_fie	-2.165017e-01	1.910925e-02	-11.329679	1.238479e-29
mean_atomic_radius	-3.084752e-01	2.928118e-02	-10.534932	7.359091e-26
wtd_mean_atomic_radius	2.615788e+00	1.195455e-01	21.881114	1.758669e-104
wtd_gmean_atomic_radius	-2.243185e+00	1.167937e-01	-19.206387	3.167485e-81
entropy_atomic_radius	5.822088e+01	1.877687e+01	3.100669	1.934459e-03
wtd_entropy_atomic_radius	4.790594e+01	4.296646e+00	11.149613	9.358693e-29
range_atomic_radius	2.009292e-01	2.558878e-02	7.852238	4.365621e-15
wtd_range_atomic_radius	-7.278254e-02	1.402750e-02	-5.188560	2.147217e-07
std_atomic_radius	-6.128447e-01	6.689823e-02	-9.160851	5.812090e-20
mean_Density	-4.480183e-03	3.008575e-04	-14.891379	8.586845e-50
wtd_gmean_Density	3.059249e-03	2.658796e-04	11.506144	1.655462e-30
entropy_Density	1.195910e+01	3.521059e+00	3.396451	6.844513e-04
wtd_entropy_Density	-1.550126e+01	2.182606e+00	-7.102183	1.283896e-12
...	...	...	...	...
std_Density	0.004645433	6.156693e-04	7.545338	4.773036e-14
wtd_mean_ElectronAffinity	0.444801766	4.037218e-02	11.017532	4.044041e-28
gmean_ElectronAffinity	0.097637435	1.697151e-02	5.753020	8.939361e-09
wtd_gmean_ElectronAffinity	-0.496111264	3.903620e-02	-12.709005	8.201160e-37
wtd_entropy_ElectronAffinity	-23.118127916	2.111158e+00	-10.950450	8.449320e-28
range_ElectronAffinity	-0.375816017	1.951690e-02	-19.255925	1.247264e-81
wtd_range_ElectronAffinity	-0.151573244	2.071458e-02	-7.317226	2.661338e-13
std_ElectronAffinity	1.167573388	5.505319e-02	21.208097	2.313411e-98
wtd_std_ElectronAffinity	-0.487420378	3.711462e-02	-13.132839	3.532710e-39
mean_FusionHeat	1.126154888	1.465822e-01	7.682753	1.654296e-14
wtd_mean_FusionHeat	-1.251994592	1.291738e-01	-9.692329	3.781446e-22
gmean_FusionHeat	-0.914910741	1.373907e-01	-6.659190	2.850288e-11
wtd_gmean_FusionHeat	0.879896513	1.136960e-01	7.739031	1.066211e-14
entropy_FusionHeat	-12.100089061	2.917463e+00	-4.147469	3.380434e-05
wtd_entropy_FusionHeat	23.200657150	2.014409e+00	11.517352	1.455366e-30
range_FusionHeat	-0.324703392	3.267521e-02	-9.937300	3.385719e-23
wtd_range_FusionHeat	0.631778738	6.687169e-02	9.447627	3.974182e-21
wtd_mean_ThermalConductivity	0.484853905	1.978383e-02	24.507591	4.679482e-130
gmean_ThermalConductivity	-0.099764034	1.551199e-02	-6.431413	1.302971e-10
wtd_gmean_ThermalConductivity	-0.298038004	1.732214e-02	-17.205611	1.046698e-65
entropy_ThermalConductivity	9.471565781	1.403489e+00	6.748586	1.548319e-11

[ ]: