

# Key to format in properties6.dat

This inscrutable format evolved over about a decade, and is naively read in by the FORTRAN code (`fetchpro6.for`) using unforgiving fixed format.

The basic materials list and coefficients for calculating the density correction are from in R. M. Sternheimer, M. J. Berger, and S. M. Seltzer, Atomic Data and Nuclear Data Tables **30**, 261-271 (1984). Compositions may be found in Int. J. Appl. Radiat. Isot. **35**, 665(1984). Also see D. E. Groom, N. V. Mokhov and S. I. Striganov, Atomic Data and Nuclear Data Tables **78**, 183-356 (2001). Updated densities, new materials, and additional properties have been added as required and requested.

The format is explained in detail in `properties6.common`.

Typical entries for an element and a compound:

9	Fluor	7	18.9984032000	5	0.47372	1.5803E-03	1.5803E-03	D	1	1	5	E
F	Fluorine gas (F%2#)											
115.0	10.9653	1.8433	4.4096	0.11083	3.2962	0.00						
9	1.000000	1.000000										
Melting point					-219.62							
Boiling point					-188.12							
Index ref (n-1)					195.							
Note: This stuff is really, really noxious. It is a pale greenish yellow gas, and forms tightly bound compounds. Note that I mark a continuation line by 5 blanks at the start.												
113	Ba-F2	5	-1.0000000000	0.42207	4.8900E+00	4.8930E+00	S	2	2	3	I	
	Barium fluoride (BaF%2#)											
375.9	5.4122	-0.0098	3.3871	0.15991	2.8867	0.00						
9	2.000000	0.216720										
56	1.000021	0.783280										
Melting point (C)					1368.							
Boiling point (C)					2260.							
Index of ref					1.4744		CRC2006	10-246				

Wrap to 150 columns OK

Separator line

12345678911234567892123456789312345678941234567895123456789612345678971234567898

## Examples of first lines:

9	Fluor	7	18.9984032000	5	0.47372	1.5803E-03	1.5803E-03	D	1	1	5	E
113	Ba-F2	5	-1.0000000000	0.42207	4.8900E+00	4.8930E+00	S	2	2	3	I	

Sternheimer index (now extended). Invisible but used by code. → 9  
 Truncated Sternheimer label (not used) → Fluor  
 Significant figures in atomic weight if element → 7  
 Atomic weight if element → 18.9984032000  
 Error in last place → 5  
 <Z/A> → 113  
 Sternheimer's density → 0.47372  
 Corrected density → 1.5803E-03  
 S(olid), L(iquid), G(as), D(iatomic gas) → 1.5803E-03  
 Elements in material → D  
 Number of optional lines → 1  
 Atoms of element 1 → 1  
 Material type: E(lement), R(adioactive element), I(norganic compound), O(rganic compound), P(olymer), M(ixture), B(iological, for dosimetry) → 5 E

**Second line:** Chemical symbol, name, and formula. "%2#" means "subscript 2", to be interpreted appropriately for TeX and for html.

F	Fluorine gas (F%2#)
	Barium fluoride (BaF%2#)

Chemical symbol if element → F  
 Name and formula; can be up to 75 characters long → Fluorine gas (F%2#)  
 Name and formula; can be up to 75 characters long → Barium fluoride (BaF%2#)

**Third line:** Mean excitation energy and Sternheimer density effect coefficients at Sternheimer's density. If  $\bar{C} = 0$  the code will construct the coefficients, but with less resulting accuracy for the density correction than if they are obtained from the ancient papers.

375.9	5.4122	-0.0098	3.3871	0.15991	2.8867	0.00
175.3	0.0	0.0000	0.0000	0.0	0.0000	0.00
$I_{eff}$ (in eV)	$\bar{C}$	$x_0$	$x_1$	$a$	$k$	$\delta_0$
effIeV	Cbar	x0	x1	aa	sk	dlt0

in Sternheimer  
 in properties5.common

**Line for each constituent element:** Number fraction is historical; calculated from A, Z, and weight fraction as a check. A modern A table was used, so small departures from integers occur. In the second example,  $I_{eff}$  is given (as it must be) but the others are 0.

9	1.000000	0.216720
56	2.000021	0.783280
Z	Number fraction	Weight fraction

**Optional lines for select properties:** Code treats col 1:5 as key. More properties can be added as needed. Not case sensitive.

Melting point (C)	1368.	Barium fluoride
Boiling point (C)	2260.	Barium fluoride BP from Rubber Bible
Index of ref	1.56	George added barium fluoride index

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**Property:** (A25) Code looks at 1:5 **Value:** F20 or E20 format **Comment:** Field starting in col 56 is not read; can be useful for records or labels.

**Optional lines for notes:** A150 format. Recognized as note if col 1:5 is 'Note:' or '. Not case sensitive. Example for polypropylene:

Note: Chem formula wrong in Sternheimer. <i>I</i> and density effect constants for polyethylene are scaled with density and used for these calculations.

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**WARNING:** Read-in code (`fetchpro6.for`) learns the number of constituent elements and number of extra property lines from the first line. If these don't agree, civilization as we know it will end.