

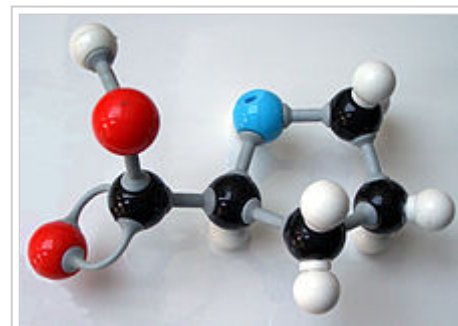
CPK coloring

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In chemistry, the **CPK coloring** is a popular color convention for distinguishing atoms of different chemical elements in molecular models. The scheme is named after the CPK molecular models designed by chemists Robert Corey and Linus Pauling, and improved by Walter Koltun.

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A plastic ball-and-stick model of proline. These models usually comply with CPK coloring.

History

In 1952, Corey and Pauling published a description of space-filling models of proteins and other biomolecules that they had been building at Caltech.^[1] Their models represented atoms by faceted hardwood balls, painted in different bright colors to indicate the respective chemical elements. Their color schema included

- White for hydrogen
- Black for carbon
- Sky blue for nitrogen
- Red for oxygen

They also built smaller models using plastic balls with the same color schema.

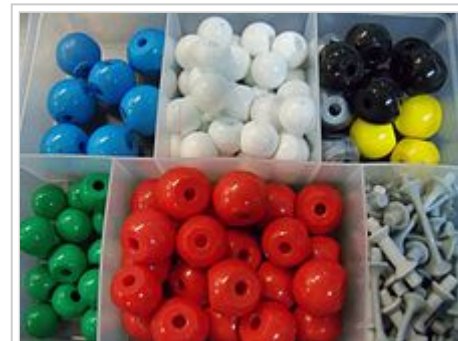
In 1965 Koltun patented an improved version of the Corey and Pauling modeling technique.^[2] In his patent he mentions the following colors:

- White for hydrogen
- Black for carbon
- Blue for nitrogen
- Red for oxygen
- Deep yellow for sulfur
- Purple for phosphorus
- Light, medium, medium dark, and dark green for the halogens (F, Cl, Br, I)
- Silver for metals (Co, Fe, Ni, Cu)

Typical assignments

Typical CPK color assignments include:

<input type="checkbox"/>	hydrogen (H)	white
<input type="checkbox"/>	carbon (C)	black
<input type="checkbox"/>	nitrogen (N)	dark blue
<input type="checkbox"/>	oxygen (O)	red
<input type="checkbox"/>	fluorine (F), chlorine (Cl)	green
<input type="checkbox"/>	bromine (Br)	dark red
<input type="checkbox"/>	iodine (I)	dark violet
<input type="checkbox"/>	noble gases (He, Ne, Ar, Xe, Kr)	cyan
<input type="checkbox"/>	phosphorus (P)	orange
<input type="checkbox"/>	sulfur (S)	yellow
<input type="checkbox"/>	boron (B), most transition metals	peach, salmon
<input type="checkbox"/>	alkali metals (Li, Na, K, Rb, Cs, Fr)	violet
<input type="checkbox"/>	alkaline earth metals (Be, Mg, Ca, Sr, Ba, Ra)	dark green
<input type="checkbox"/>	titanium (Ti)	gray
<input type="checkbox"/>	iron (Fe)	orange
<input type="checkbox"/>	other elements	pink



A box of ball-and-stick model pieces colored to represent several of the common elements.

Several of the CPK colors refer mnemonically to colors of the pure elements or notable compound. For example, hydrogen is a colorless gas, carbon as charcoal or graphite is black, common sulfur is yellow, chlorine is a greenish gas, bromine is a dark red liquid, iodine in ether is violet, amorphous phosphorus is red, rust is dark orange-red, etc. For some colors, such as those of oxygen and nitrogen, the inspiration is less clear. Perhaps red for oxygen is inspired by the fact that oxygen is normally required for combustion or that the oxygen-bearing chemical in blood, hemoglobin, is bright red, and the blue for nitrogen by the fact that nitrogen is the main component of Earth's atmosphere, which appears to human eyes as being colored sky blue.

Modern variants

The following table shows colors assigned to each element by some popular software products. Column **C** is the original assignment by Corey and Pauling,^[1] and **K** is that of Koltun's patent.^[2] Column **J** is the color scheme used by the molecular visualizer Jmol.^[3] Column **R** is the scheme used by Rasmol; when two colors are shown, the second one is valid for versions 2.7.3 and later.^{[3][4]} All colors are approximate and may depend on the display hardware and viewing conditions.

A#	Sy	Element	Colors			
			C	K	J	R
1	H	hydrogen	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
1	² H (D)	deuterium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
1	³ H (T)	tritium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
2	He	helium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
3	Li	lithium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
4	Be	beryllium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
5	B	boron	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
6	C	carbon	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
6	¹³ C	carbon 13	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
6	¹⁴ C	carbon 14	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
7	N	nitrogen	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
7	¹⁵ N	nitrogen 15	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
8	O	oxygen	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
9	F	fluorine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
10	Ne	neon	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
11	Na	sodium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
12	Mg	magnesium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
13	Al	aluminium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
14	Si	silicon	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
15	P	phosphorus	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
16	S	sulfur	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
17	Cl	chlorine	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
18	Ar	argon	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
19	K	potassium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
20	Ca	calcium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
21	Sc	scandium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
22	Ti	titanium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
23	V	vanadium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
24	Cr	chromium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
25	Mn	manganese	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
26	Fe	iron	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
27	Co	cobalt	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
28	Ni	nickel	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
29	Cu	copper	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
30	Zn	zinc	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
31	Ga	gallium	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

32	Ge	germanium			<input type="checkbox"/>	<input type="checkbox"/>
33	As	arsenic			<input type="checkbox"/>	<input type="checkbox"/>
34	Se	selenium			<input type="checkbox"/>	<input type="checkbox"/>
35	Br	bromine		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
36	Kr	krypton			<input type="checkbox"/>	<input type="checkbox"/>
37	Rb	rubidium			<input type="checkbox"/>	<input type="checkbox"/>
38	Sr	strontium			<input type="checkbox"/>	<input type="checkbox"/>
39	Y	yttrium			<input type="checkbox"/>	<input type="checkbox"/>
40	Zr	zirconium			<input type="checkbox"/>	<input type="checkbox"/>
41	Nb	niobium			<input type="checkbox"/>	<input type="checkbox"/>
42	Mo	molybdenum			<input type="checkbox"/>	<input type="checkbox"/>
43	Tc	technetium			<input type="checkbox"/>	<input type="checkbox"/>
44	Ru	ruthenium			<input type="checkbox"/>	<input type="checkbox"/>
45	Rh	rhodium			<input type="checkbox"/>	<input type="checkbox"/>
46	Pd	palladium			<input type="checkbox"/>	<input type="checkbox"/>
47	Ag	silver			<input type="checkbox"/>	<input type="checkbox"/>
48	Cd	cadmium			<input type="checkbox"/>	<input type="checkbox"/>
49	In	indium			<input type="checkbox"/>	<input type="checkbox"/>
50	Sn	tin			<input type="checkbox"/>	<input type="checkbox"/>
51	Sb	antimony			<input type="checkbox"/>	<input type="checkbox"/>
52	Te	tellurium			<input type="checkbox"/>	<input type="checkbox"/>
53	I	iodine		<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
54	Xe	xenon			<input type="checkbox"/>	<input type="checkbox"/>
55	Cs	caesium			<input type="checkbox"/>	<input type="checkbox"/>
56	Ba	barium			<input type="checkbox"/>	<input type="checkbox"/>
57	La	lanthanum			<input type="checkbox"/>	<input type="checkbox"/>
58	Ce	cerium			<input type="checkbox"/>	<input type="checkbox"/>
59	Pr	praseodymium			<input type="checkbox"/>	<input type="checkbox"/>
60	Nd	neodymium			<input type="checkbox"/>	<input type="checkbox"/>
61	Pm	promethium			<input type="checkbox"/>	<input type="checkbox"/>
62	Sm	samarium			<input type="checkbox"/>	<input type="checkbox"/>
63	Eu	europium			<input type="checkbox"/>	<input type="checkbox"/>
64	Gd	gadolinium			<input type="checkbox"/>	<input type="checkbox"/>
65	Tb	terbium			<input type="checkbox"/>	<input type="checkbox"/>
66	Dy	dysprosium			<input type="checkbox"/>	<input type="checkbox"/>
67	Ho	holmium			<input type="checkbox"/>	<input type="checkbox"/>
68	Er	erbium			<input type="checkbox"/>	<input type="checkbox"/>
69	Tm	thulium			<input type="checkbox"/>	<input type="checkbox"/>
70	Yb	ytterbium			<input type="checkbox"/>	<input type="checkbox"/>

71	Lu	lutetium			<input type="checkbox"/>	<input type="checkbox"/>
72	Hf	hafnium			<input type="checkbox"/>	<input type="checkbox"/>
73	Ta	tantalum			<input type="checkbox"/>	<input type="checkbox"/>
74	W	tungsten			<input type="checkbox"/>	<input type="checkbox"/>
75	Re	rhenium			<input type="checkbox"/>	<input type="checkbox"/>
76	Os	osmium			<input type="checkbox"/>	<input type="checkbox"/>
77	Ir	iridium			<input type="checkbox"/>	<input type="checkbox"/>
78	Pt	platinum			<input type="checkbox"/>	<input type="checkbox"/>
79	Au	gold			<input type="checkbox"/>	<input type="checkbox"/>
80	Hg	mercury			<input type="checkbox"/>	<input type="checkbox"/>
81	Tl	thallium			<input type="checkbox"/>	<input type="checkbox"/>
82	Pb	lead			<input type="checkbox"/>	<input type="checkbox"/>
83	Bi	bismuth			<input type="checkbox"/>	<input type="checkbox"/>
84	Po	polonium			<input type="checkbox"/>	<input type="checkbox"/>
85	At	astatine			<input type="checkbox"/>	<input type="checkbox"/>
86	Rn	radon			<input type="checkbox"/>	<input type="checkbox"/>
87	Fr	francium			<input type="checkbox"/>	<input type="checkbox"/>
88	Ra	radium			<input type="checkbox"/>	<input type="checkbox"/>
89	Ac	actinium			<input type="checkbox"/>	<input type="checkbox"/>
90	Th	thorium			<input type="checkbox"/>	<input type="checkbox"/>
91	Pa	protactinium			<input type="checkbox"/>	<input type="checkbox"/>
92	U	uranium			<input type="checkbox"/>	<input type="checkbox"/>
93	Np	neptunium			<input type="checkbox"/>	<input type="checkbox"/>
94	Pu	plutonium			<input type="checkbox"/>	<input type="checkbox"/>
95	Am	americium			<input type="checkbox"/>	<input type="checkbox"/>
96	Cm	curium			<input type="checkbox"/>	<input type="checkbox"/>
97	Bk	berkelium			<input type="checkbox"/>	<input type="checkbox"/>
98	Cf	californium			<input type="checkbox"/>	<input type="checkbox"/>
99	Es	einsteinium			<input type="checkbox"/>	<input type="checkbox"/>
100	Fm	fermium			<input type="checkbox"/>	<input type="checkbox"/>
101	Md	mendelevium			<input type="checkbox"/>	<input type="checkbox"/>
102	No	nobelium			<input type="checkbox"/>	<input type="checkbox"/>
103	Lr	lawrencium			<input type="checkbox"/>	<input type="checkbox"/>
104	Rf	rutherfordium			<input type="checkbox"/>	<input type="checkbox"/>
105	Db	dubnium			<input type="checkbox"/>	<input type="checkbox"/>
106	Sg	seaborgium			<input type="checkbox"/>	<input type="checkbox"/>
107	Bh	bohrium			<input type="checkbox"/>	<input type="checkbox"/>
108	Hs	hassium			<input type="checkbox"/>	<input type="checkbox"/>
109	Mt	meitnerium			<input type="checkbox"/>	<input type="checkbox"/>

110	Ds	darmstadtium				<input type="checkbox"/>
111	Rg	roentgenium				<input type="checkbox"/>
112	Cn	copernicium				<input type="checkbox"/>
113	Uut	ununtrium				<input type="checkbox"/>
114	Fl	flerovium				<input type="checkbox"/>
115	Uup	ununpentium				<input type="checkbox"/>
116	Lv	livermorium				<input type="checkbox"/>
117	Uus	ununseptium				<input type="checkbox"/>
118	Uuo	ununoctium				<input type="checkbox"/>

See also

- Molecular graphics
- Ball-and-stick model
- Software for molecular modeling

References

1. Robert B. Corey and Linus Pauling (1953): Molecular Models of Amino Acids, Peptides, and Proteins. Review of Scientific Instruments, Volume 24, Issue 8, pp. 621-627. doi:10.1063/1.1770803 (<https://dx.doi.org/10.1063%2F1.1770803>)
2. Walter L. Koltun (1965), *Space filling atomic units and connectors for molecular models*. U. S. Patent 3170246.
3. Jmol color table (<http://jmol.sourceforge.net/jscolors/>) at sourceforge.net. Accessed on 2010-01-28.
4. Rasmol color table (<http://www.bio.cmu.edu/Courses/BiochemMols/RasFrames/CPKCLRS.HTM>) at bio.cmu.edu. Accessed on 2010-01-28.

External links

- What is the basis for the CPK color scheme? Which colors is used for which atom? (<http://www.biosino.org/mirror/www.ncbi.nlm.nih.gov/Structure/cn3d/cn3dfaq.html#colorCPK>)
- Physical Molecular Models (<http://www.netsci.org/Science/Compchem/feature14b.html>)

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Categories: Molecular modelling | Colors

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