

Welcome to 3.091

Lecture 11
October 2, 2009

The Shapes of Molecules

3.091 Test #1

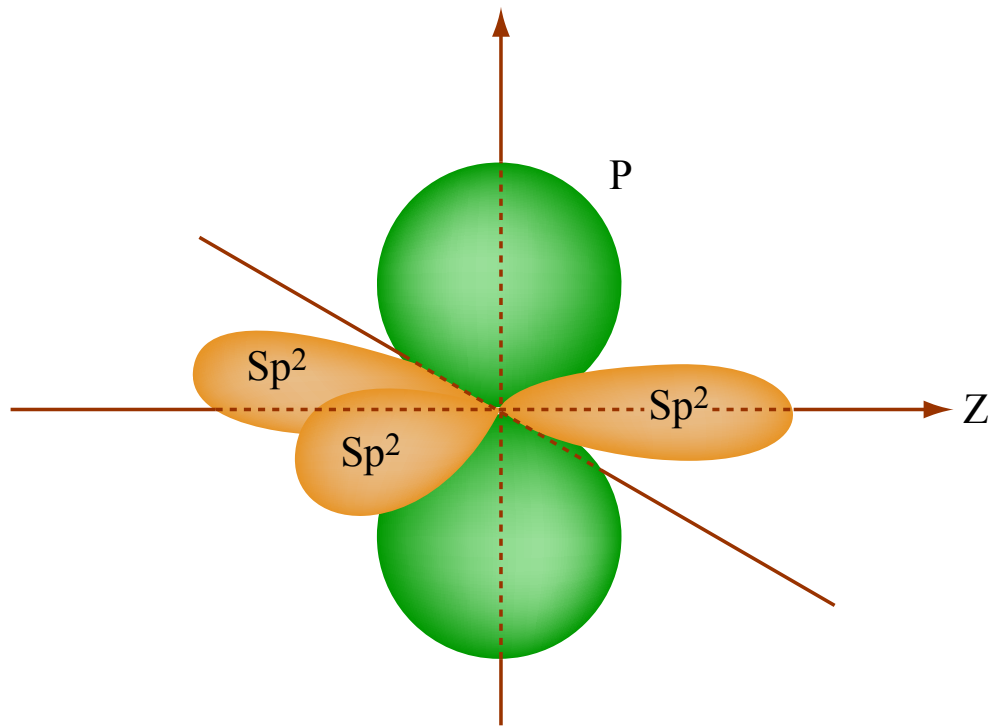
Wednesday, October 7, 2009

Room Assignments

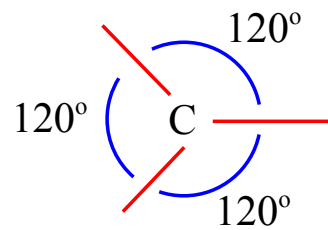
A – Ha: 10-250

He - Sm: 26-100

So - ∞ : 4-270



Top View



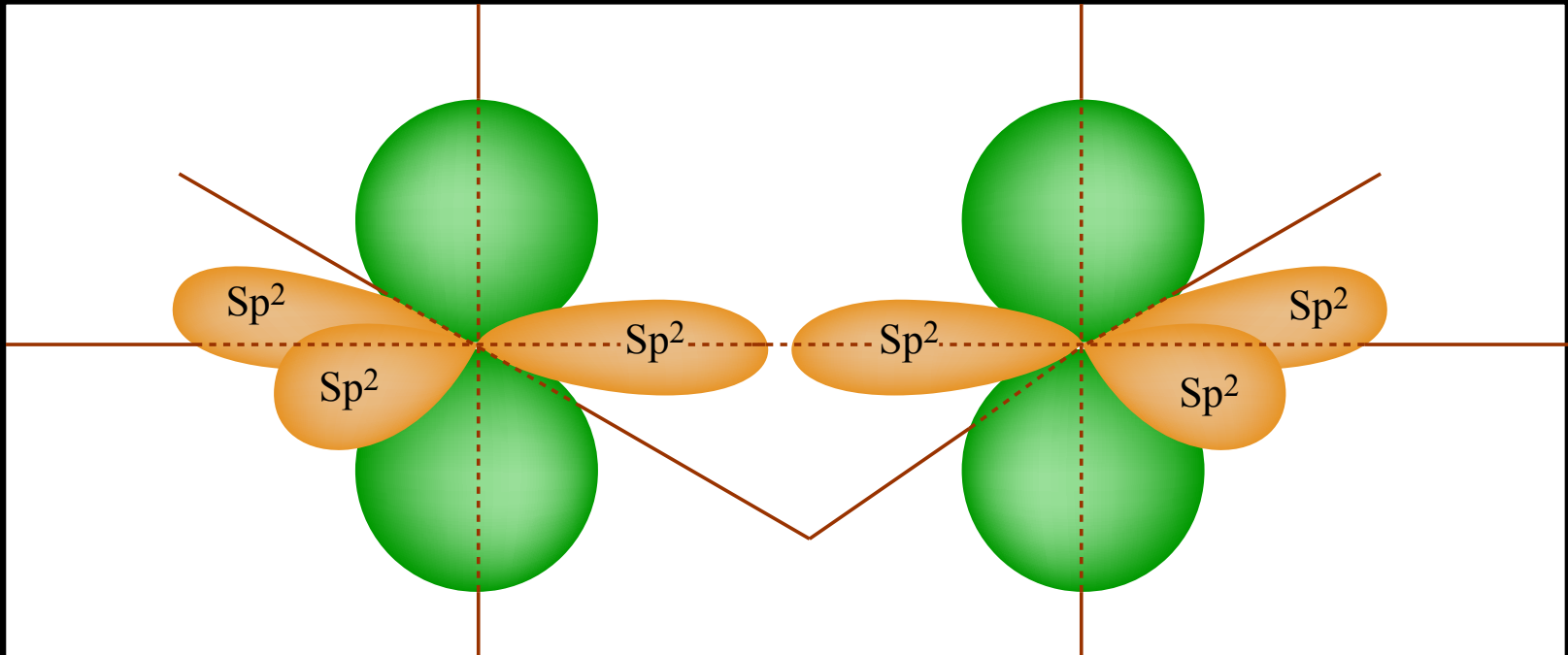


Image by MIT OpenCourseWare.

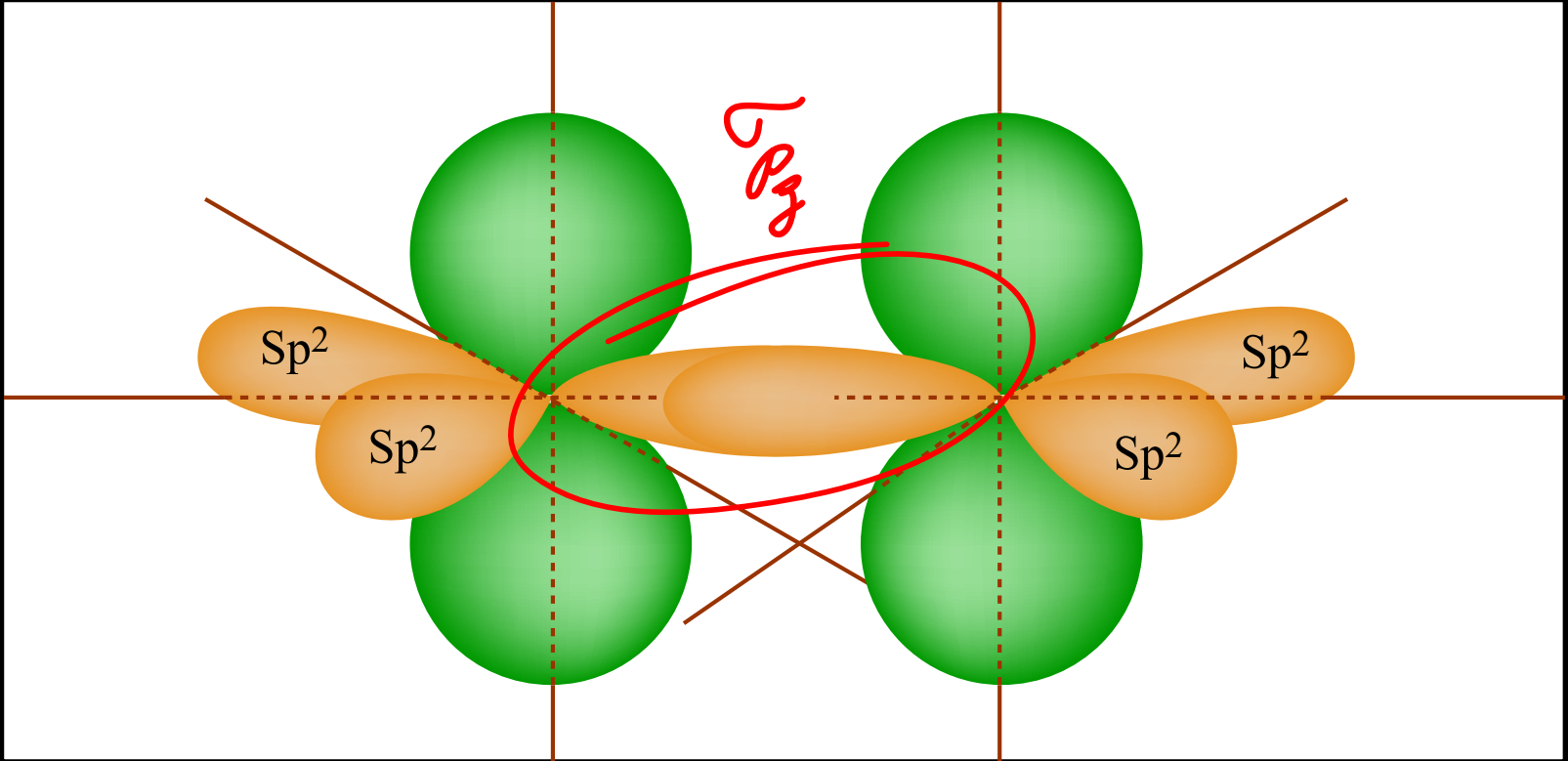


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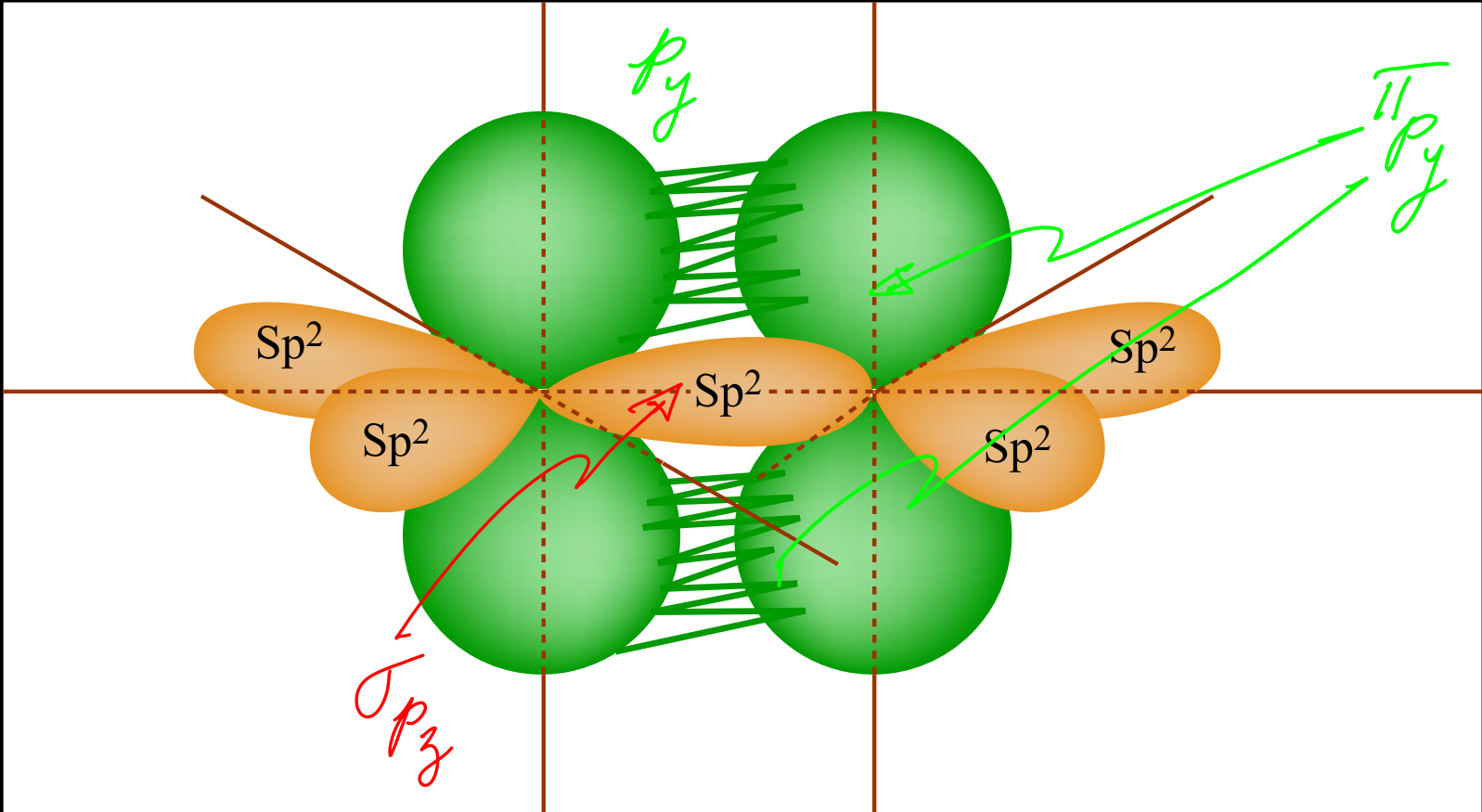


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C₂H₄ pi bonding

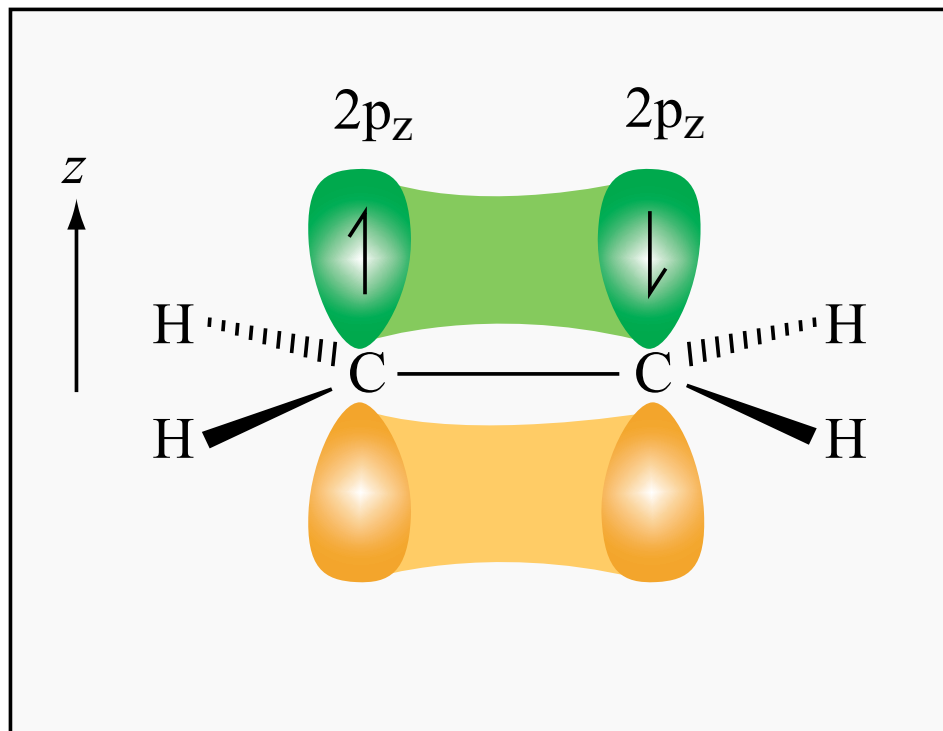
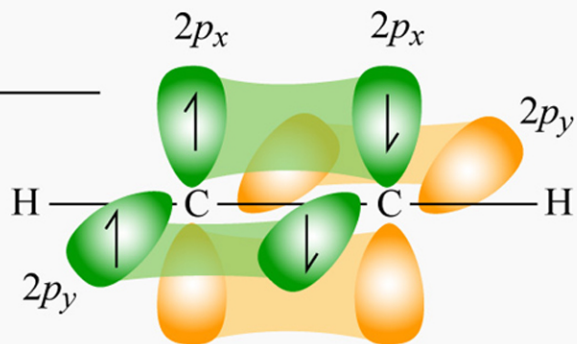
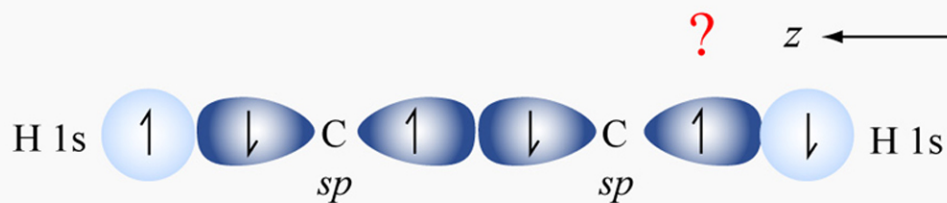


Image by MIT OpenCourseWare.

ethylene C₂H₄

(a) C_2H_2 sigma-bonded framework

(b) C_2H_2 pi bonding



acetylene C_2H_2

Image by MIT OpenCourseWare.

acetylene C_2H_2

Rules for Determining Molecular Shape: Valence-Shell Electron-Pair-Repulsion Model

1. write the Lewis structure \Rightarrow electron distribution
 \Rightarrow molecular skeleton
2. classify each electron pair as bonding (B) or nonbonding (NB)
3. maximize separation between domains
4. give more space to NB domains and to B domains comprising multiple bonds (EPR)
5. place NB domains at equatorial positions in a trigonal bipyramid

Element capable of expanded octet

Electron Configuration

1A																	8A
H																	He
2A												3A	4A	5A	6A	7A	
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
		3B	4B	5B	6B	7B	8B			1B	2B						
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub						

→ good e⁻ acceptors

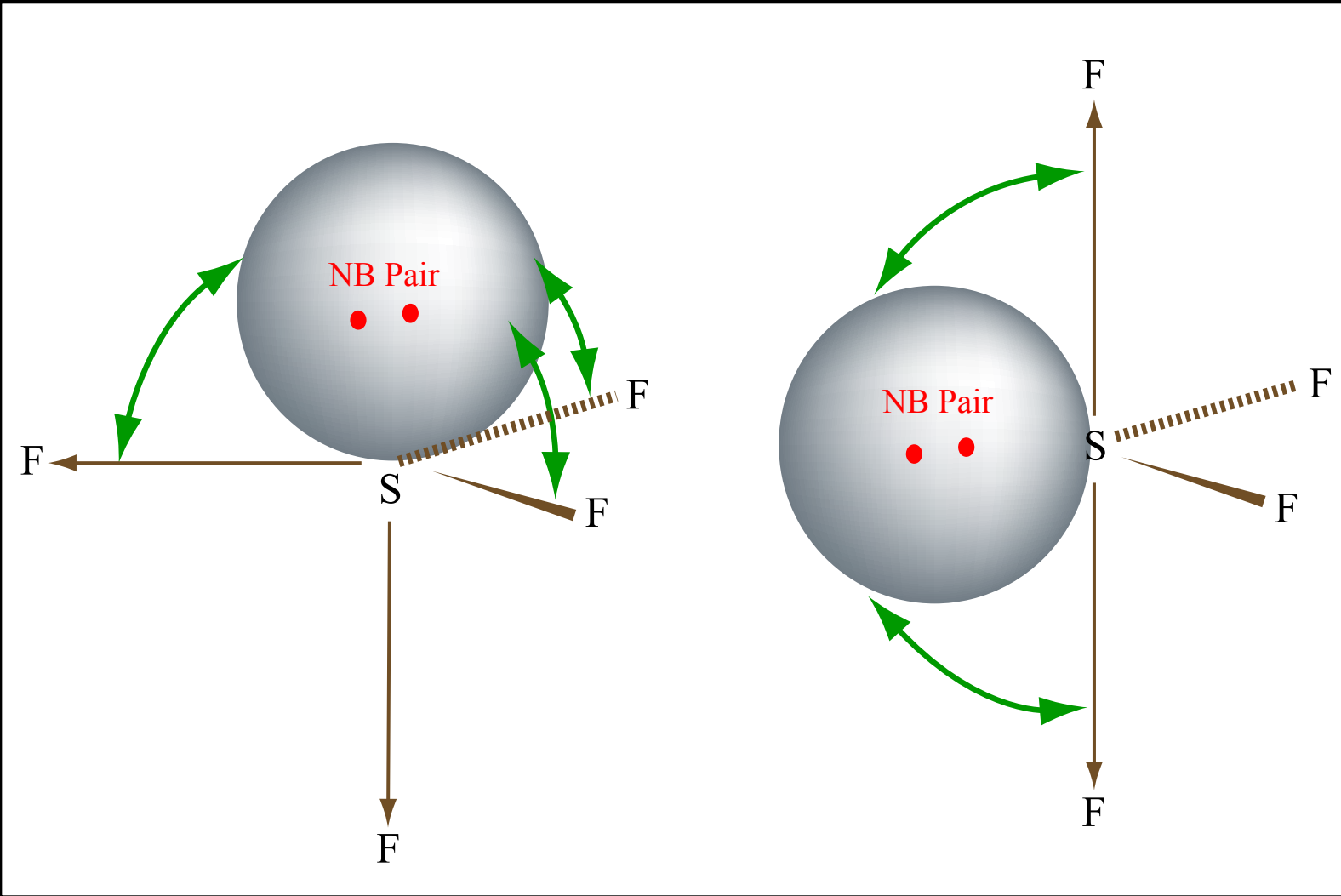


Image by MIT OpenCourseWare.

Electron-pair geometries for species with two to six electron pairs


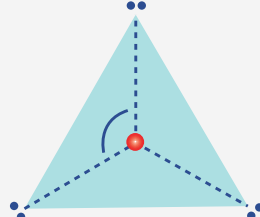
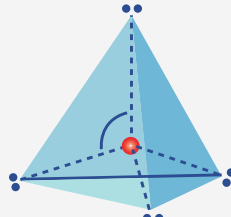
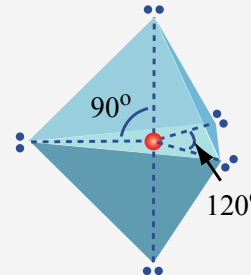
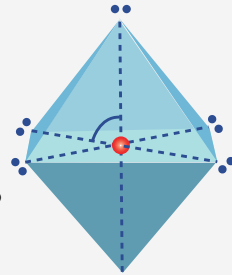

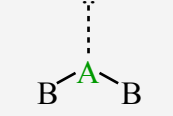
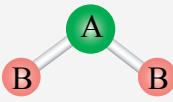
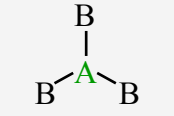
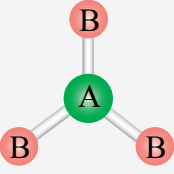
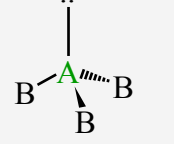
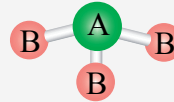
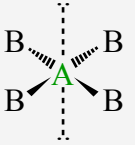
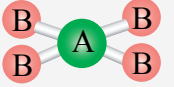
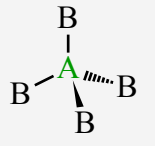
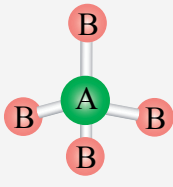
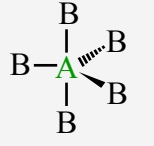
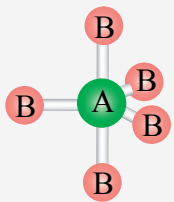
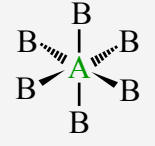
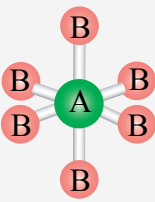
Electron pairs	2	3	4	5	6
Geometry	Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
					
Predicted bond angles	180°	120°	109.5°	$90^\circ, 120^\circ$	90°

Image by MIT OpenCourseWare.

Common molecular geometries for species with two to six bonded atoms^a

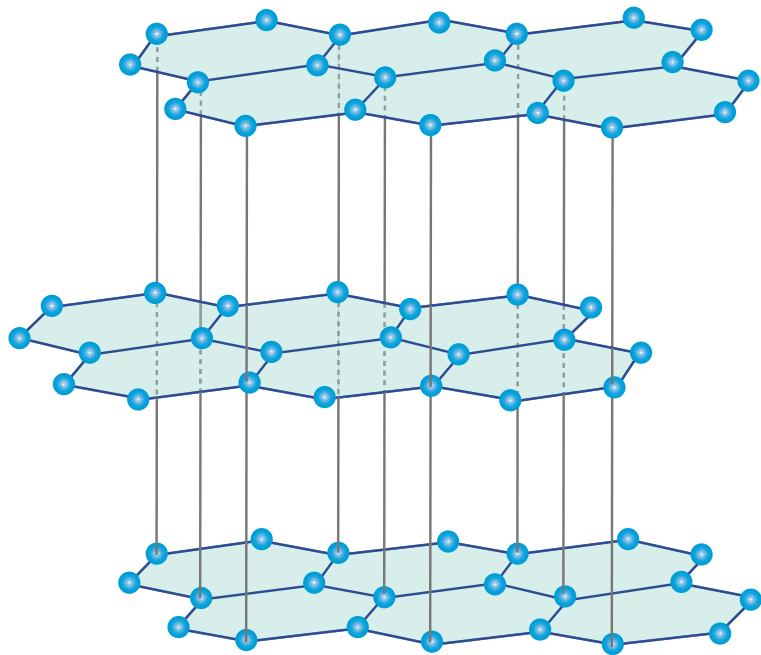
AB_n Notation	AB_2	AB_2	AB_3	AB_3
Geometry	Linear	Bent (V-shaped)	Trigonal planar	Trigonal pyramidal
	$B-A-B$ 	 	 	 
Idealized bond angles	180°	$<180^\circ$	120°	$<120^\circ$
AB_n Notation	AB_4	AB_4	AB_5	AB_6
Geometry	Square planar	Tetrahedral	Trigonal bipyramidal	Octahedral
	 	 	 	 
Idealized bond angles	90°	109.5°	$90^\circ, 120^\circ$	90°

^a Lone pairs are shown using a dashed line.

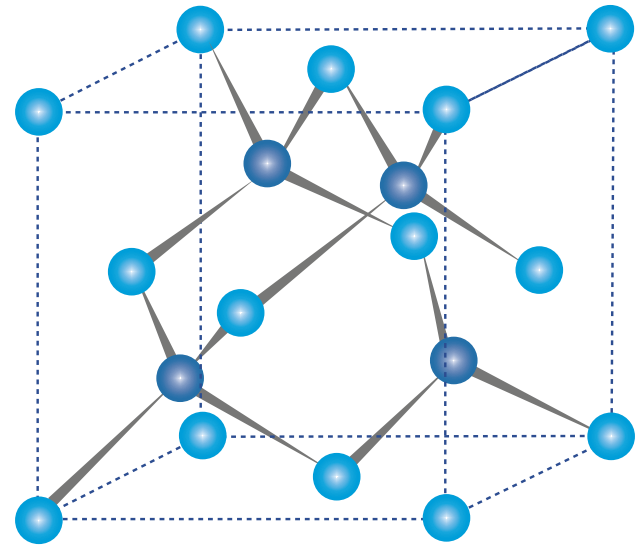
Overview of molecular geometries

Electron pairs	2	3	4	5	6
Electron pairs geometry					
	Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
Molecular geometry: Zero lone pairs					
	Linear AB ₂	Trigonal planar AB ₃	Tetrahedral AB ₄	Trigonal bipyramidal AB ₅	Octahedral AB ₆
Molecular geometry: One lone pair					
		Bent (V-shaped) AB ₂	Trigonal pyramidal AB ₃	Seesaw AB ₄	Square pyramidal AB ₅
Molecular geometry: Two lone pairs					
			Bent (V-shaped) AB ₂	T-shaped AB ₃	Square planar AB ₄
Molecular geometry: Three lone pairs					
				Linear AB ₂	

Graphite



Diamond



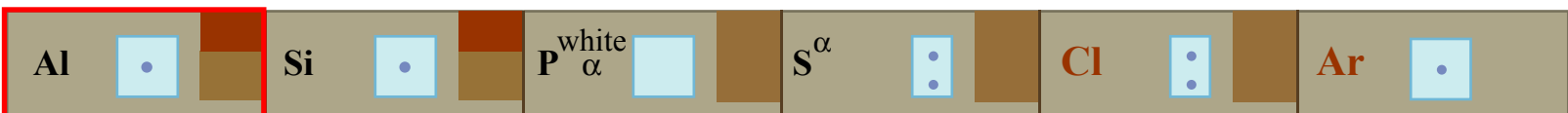


0.31	-
-	0.0829
31.8	-
1.34/0.2050	5.193
-	0.001520

What's the stable form of C?



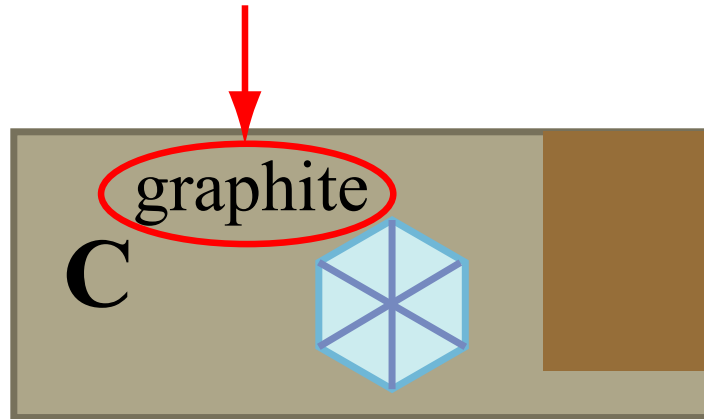
0.82	22.18	0.77	104.60	0.75	0.3605	0.73	0.2224	0.72	0.255	0.71	0.3347
0.98	480	0.91	716.72 ^{ES}	0.92/[1.5]	2.79	[1.40]	3.41	[1.35]	3.31	-	1.71
4.68	573.21	5.34	-	17.3	472.79	14.0	249.37	17.1	79.08	16.8	-
1.56/3.03	1.026	1.82/1.76	0.709	2.07/1.10	1.040	2.00/0.802	0.918	2.26/0.557	0.824	2.52/0.3956	1.030
-	0.274	-	1.2-1.5	-	0.0002598	-	0.0002575	-	0.000279	-	0.000493*



1.18	10.669	1.11	46.44	1.06	0.628	1.02	1.72	0.99	3.38	0.98	1.176
1.43	293.72	1.32	439	1.28/[1.9]	12.43	1.27/[1.85]	9.62	[1.80]	10.21	-	6.43
9.99	322.17	12.05	439.32	17.0	314.64	15.5	278.65	18.7	121.75	24.2	-
1.99/6.8	0.897	2.32/5.38	0.705	2.63/3.63	0.769	2.62/2.90	0.710	2.93/2.18	0.479	3.23/1.6411	0.520
2.709	2.37	-	1.49	-	0.00236*	-	0.00270	-	0.000089	-	0.0001772

13 IIIB IIIA	14 IVB IVA	15 VB VA	16 VIB VIA	17 VIIB VIIA	18 VIII 0
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Not diamond!



0.77	104.60
0.91	716.72 ^{ES}
5.34	-
1.82/1.76	0.709
-	1.2-1.5

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3.091SC Introduction to Solid State Chemistry
Fall 2009

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