









VSEPR and Molecular Geometries











Common molecular geometries

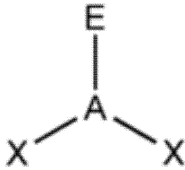
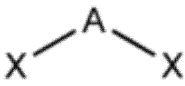
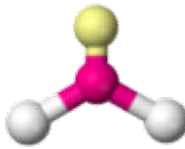

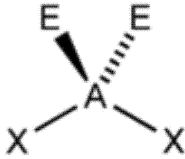
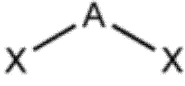
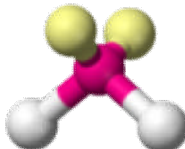

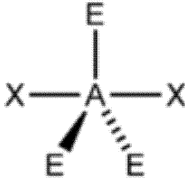

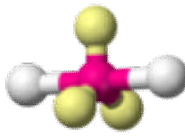

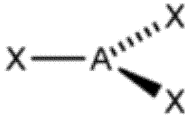
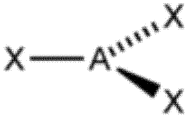
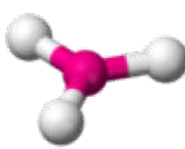
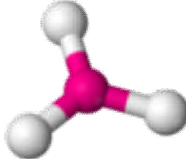
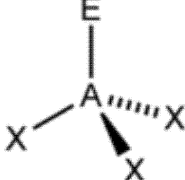

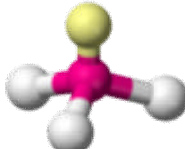
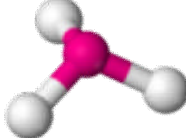
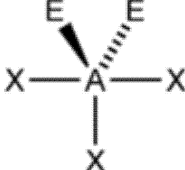
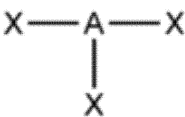
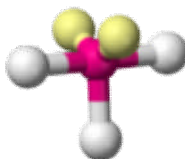
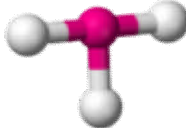
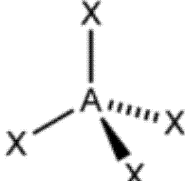
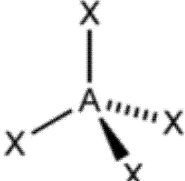
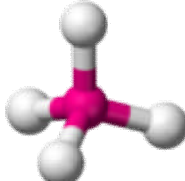
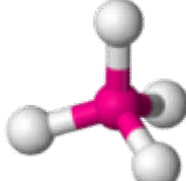
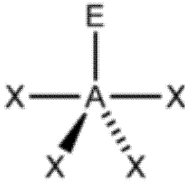

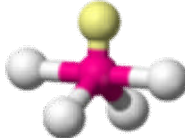

 linear	 bent	 trigonal planar	 pyramidal
 square planar	 tetrahedral	 trigonal bipyramidal	 octahedral

Molecular geometry and lone pairs

You can use the so-called *AXE method* to calculate the shape of a molecule. It is based on molecules that have a central atom, which we label A. Atoms or groups bonded to A are labelled X. Lone pairs are labelled E. A molecule with three lone pairs and two atoms/groups bonded to it would be denoted AX_2E_3 . The table below shows how X and E and molecular shape are related.

Valence shell electron pair repulsion theory (VSEPR) is used to predict the shape of a molecule once X and E are known. This sounds more complicated than it is. You consider any X's and E's to be regions of charge that position themselves as far apart from each other as possible, in order to minimize the forces of electrostatic repulsion between each other.

AXE label	X (substituents)	E (lone pairs)	Shape	2D diagram lone pairs shown	2D diagram lone pairs not shown	3D model lone pairs shown	3D model lone pairs not shown	Examples
AX_1E_0	1	0	Linear	$A-X$	$A-X$			HF O ₂
AX_1E_1	1	1	Linear	$E-A-X$	$A-X$			CN ⁻
AX_1E_2	1	2	Linear	$\begin{array}{c} E \\ \diagdown \\ A-X \\ \diagup \\ E \end{array}$	$A-X$			H ₂ CO
AX_1E_3	1	3	Linear	$\begin{array}{c} E \\ \diagdown \\ A-X \\ \diagup \\ E \\ \diagup \\ E \end{array}$	$A-X$			HCl
AX_2E_0	2	0	Linear	$X-A-X$	$X-A-X$			BeCl ₂ HgCl ₂ CO ₂

AXE label	X (substituents)	E (lone pairs)	Shape	2D diagram lone pairs shown	2D diagram lone pairs not shown	3D model lone pairs shown	3D model lone pairs not shown	Examples
AX_2E_1	2	1	Bent					NO_2^- SO_2 O_3
AX_2E_2	2	2	Bent					H_2O H_2S OF_2
AX_2E_3	2	3	Linear					XeF_2 I_3^-
AX_3E_0	3	0	Trigonal planar					BF_3 CO_3^{2-} NO_3^- SO_3
AX_3E_1	3	1	Trigonal pyramidal					NH_3 PCl_3
AX_3E_2	3	2	T-shaped					ClF_3 BrF_3
AX_4E_0	4	0	Tetrahedral					CH_4 NH_4^+ PO_4^{3-} SO_4^{2-} ClO_4^-
AX_4E_1	4	1	Seesaw					SF_4

AXE label	X (substituents)	E (lone pairs)	Shape	2D diagram lone pairs shown	2D diagram lone pairs not shown	3D model lone pairs shown	3D model lone pairs not shown	Examples
AX_4E_2	4	2	Square Planar					XeF_4
AX_5E_0	5	0	Trigonal Bipyramidal					PCl_5
AX_5E_1	5	1	Square Pyramidal					ClF_5 BrF_5
AX_6E_0	6	0	Octahedral					SF_6
AX_6E_1	6	1	Pentagonal pyramidal					XeF_6
AX_7E_0	7	0	Pentagonal bipyramidal					