

Minimum energy arrangements of electron pair groups to determine Molecular Geometries

Arranged by electron domain number (N)

Note that when L=0 the framework geometry is the same as the molecular geometry

type	N	B	L	Framework geometry	Molecular geometry	Comment	Examples
AX ₂	2	2	0	Linear	Linear	The angle X-A-X is exactly 180°	BeH ₂ , CO ₂ , HCN
AX ₃	3	3	0	Trigonal planar	Trigonal planar	If the molecule is symmetric then the X-A-X angles are all exactly 120°; if the atoms X differ, as in H ₂ CO, then these angles may differ slightly from 120°, but all four atoms still lie strictly in a plane	BF ₃ , SO ₃ , NO ₃ ⁻ , CO ₃ ²⁻ , H ₂ CO
AX ₂	3	2	1	Trigonal planar	Bent	The angle X-A-X is << 180°, usually about 120°	O ₃ , SO ₂ , NO ₂ ⁻
AX ₄	4	4	0	Tetrahedral	Tetrahedral	If the molecule is symmetric then the X-A-X angles are all 109.47°; If the atoms X differ, as in CH ₂ Cl ₂ , then these angles may differ slightly from 109.47°. This tetrahedral arrangement is NOT planar.	CCl ₄ , CH ₂ Cl ₂ , NH ₄ ⁺ , SO ₄ ²⁻ , S ₂ O ₃ ²⁻
AX ₃	4	3	1	Tetrahedral	Trigonal pyramidal	Angle X-A-X is slightly less than 109.47°. This arrangement is NOT planar	NH ₃ , PCl ₃ , H ₃ O ⁺ , XeO ₃
AX ₂	4	2	2	Tetrahedral	Bent	The angle X-A-X is slightly less than the tetrahedral angle, 109.47°	H ₂ O, H ₂ S
AX ₅	5	5	0	TBP = Trigonal bipyramidal	TBP	Two X axial, 180° apart; three X equatorial, 120° apart; angle X _{ax} -X _{eq} 90°	PCl ₅
AX ₄	5	4	1	TBP	Seesaw	Lone pairs are found in equatorial positions, since these have more space.	SF ₄
AX ₃	5	3	2	TBP	T-shaped	Lone pairs in equatorial positions.	ClF ₃ , C ₆ H ₅ ICl ₂
AX ₂	5	2	3	TBP	Linear	Lone pairs in equatorial positions	I ₃ ⁻ , XeF ₂
AX ₆	6	6	0	Octohedral	Octohedral	All X-A-X angles are 90° [<i>cis</i>] or 180° [<i>trans</i>]	SF ₆ , PF ₆ ⁻ , Te(OH) ₆
AX ₅	6	5	1	Octohedral	Square pyramid		BrF ₅
AX ₄	6	4	2	Octohedral	Square planar	Lone pairs opposite, since they take more space	XeF ₄
AX ₇	7	7	0	Pentagonal bipyramidal	Pentagonal bipyramidal		IF ₇

Minimum energy arrangements of electron pair groups to predict Molecular Geometries

Arranged by fragment type (equivalently, by B)

type	N	B	L	Framework geometry	Molecular geometry	Comment	Examples
AX ₂	2	2	0	Linear	Linear	The angle X-A-X is exactly 180°	BeH ₂ , CO ₂ , HCN
AX ₂	3	2	1	Trigonal planar	Bent	The angle X-A-X is << 180°, usually about 120°	O ₃ , SO ₂ , NO ₂ ⁻
AX ₂	4	2	2	Tetrahedral	Bent	The angle X-A-X is slightly less than the tetrahedral angle, 109.47°	H ₂ O, H ₂ S
AX ₂	5	2	3	TBP = Trigonal bipyramidal	Linear	Lone pairs are found in equatorial positions, since these have more space	I ₃ ⁻ , XeF ₂
AX ₃	3	3	0	Trigonal planar	Trigonal planar	If the molecule is symmetric then the X-A-X angles are all exactly 120°; if the atoms X differ, as in H ₂ CO, then these angles may differ slightly from 120°, but all four atoms still lie strictly in a plane	BF ₃ , SO ₃ , NO ₃ ⁻ , CO ₃ ²⁻ , H ₂ CO
AX ₃	4	3	1	Tetrahedral	Trigonal pyramidal	Angle X-A-X is slightly less than 109.47°. This arrangement is NOT planar	NH ₃ , PCl ₃ , H ₃ O ⁺ , XeO ₃
AX ₃	5	3	2	TBP	T-shaped	Lone pairs in equatorial positions.	ClF ₃ , C ₆ H ₅ ICl ₂
AX ₄	4	4	0	Tetrahedral	Tetrahedral	If the molecule is symmetric then the X-A-X angles are all 109.47°; If the atoms X differ, as in CH ₂ Cl ₂ , then these angles may differ slightly from 109.47°. This tetrahedral arrangement is NOT planar.	CCl ₄ , CH ₂ Cl ₂ , NH ₄ ⁺ , SO ₄ ²⁻ , S ₂ O ₃ ²⁻
AX ₄	5	4	1	TBP	Seesaw	Lone pairs in equatorial positions	SF ₄
AX ₄	6	4	2	Octohedral	Square planar		XeF ₄
AX ₅	5	5	0		TBP	Two X axial, 180° apart; three X equatorial, 120° apart; angle X _{ax} -X _{eq} 90°	PCl ₅
AX ₅	6	5	1	Octohedral	Square pyramid		BrF ₅
AX ₆	6	6	0	Octohedral	Octohedral	All X-A-X angles are 90° [<i>cis</i>] or 180° [<i>trans</i>]	SF ₆ , PF ₆ ⁻ , Te(OH) ₆
AX ₇	7	7	0	Pentagonal bipyramidal	Pentagonal bipyramidal		IF ₇