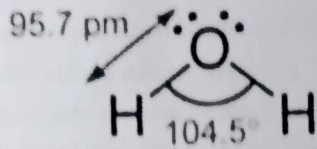


## VSEPR theory

**Valence shell electron pair repulsion (VSEPR) theory** (*V*espar, *va* sepa*r*/ *V*ESP-*er*,<sup>[1]:410</sup> *va* SEP-*er*<sup>[2]</sup>), is a model used in chemistry to predict the geometry of individual molecules from the number of electron pairs surrounding their central atoms.<sup>[3]</sup> It is also named the Gillespie-Nyholm theory after its two main developers, Ronald Gillespie and Ronald Nyholm.



Example of bent electron arrangement. Shows location of unpaired electrons, bonded atoms, and bond angles. (Water molecule)  
The bond angle for water is 104.5°.

The premise of VSEPR is that the valence electron pairs surrounding an atom tend to repel each other and will, therefore, adopt an arrangement that minimizes this repulsion. This in turn decreases the molecule's energy and increases its stability, which determines the molecular geometry. Gillespie has emphasized that the electron-electron repulsion due to the Pauli exclusion principle is more important in determining molecular geometry than the electrostatic repulsion.<sup>[4]</sup>

The insights of VSEPR theory are derived from topological analysis of the electron density of molecules. Such quantum chemical topology (QCT) methods include the electron localization function (ELF) and the quantum theory of atoms in molecules (AIM or QTAIM).<sup>[4][5]</sup> Hence, VSEPR is unrelated to wave function-based methods such as orbital hybridisation in valence bond theory.<sup>[6]</sup>

## History

The idea of a correlation between molecular geometry and number of valence electron pairs (both shared and unshared pairs) was originally proposed in 1939 by Ryutarō Tsuchida in Japan,<sup>[7]</sup> and was independently presented in a Bakerian Lecture in 1940 by Nevil Sidgwick and Herbert Powell of the University of Oxford.<sup>[8]</sup> In 1957, Ronald Gillespie and Ronald Sydney Nyholm of University College London refined this concept into a more detailed theory, capable of choosing between various alternative geometries.<sup>[9][10]</sup>

## Overview

VSEPR theory is used to predict the arrangement of electron pairs around central atoms in molecules, especially simple and symmetric molecules. A central atom is defined in this theory as an atom which is bonded to two or more other atoms, while a terminal atom is bonded to only one other atom.<sup>[1]:398</sup> For example in the molecule methyl isocyanate ( $\text{H}_3\text{C}-\text{N}=\text{C}=\text{O}$ ), the two carbons and one nitrogen are central atoms, and the three hydrogens and one oxygen are terminal atoms.<sup>[1]:416</sup> The geometry of the central atoms and their non-bonding electron pairs in turn determine the geometry of the larger whole molecule.

The number of electron pairs in the valence shell of a central atom is determined after drawing the Lewis structure of the molecule, and expanding it to show all bonding groups and lone pairs of electrons.<sup>[1]:410-417</sup> In VSEPR theory, a double bond or triple bond is treated as a single bonding group.<sup>[1]</sup> The sum of the number of atoms bonded to a central atom and the number of lone pairs formed by its nonbonding valence electrons is known as the central atom's steric number.

The electron pairs (or groups if multiple bonds are present) are assumed to lie on the surface of a sphere centered on the central atom and tend to occupy positions that minimize their mutual repulsions by maximizing the distance between