Molecular orbital theory for octahedral and tetrahedral metal complexes pdf

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 Square planar molecular geometryExamplesXeF4, PtCl2−4Point groupD4hCoordination number4Bond angle(s)90°μ (Polarity)0 Structure of cisplatin, an example of a molecule with the square planar coordination geometry. The square planar molecular geometry in chemistry describes the stereochemistry (spatial arrangement of atoms) that is adopted by certain chemical compounds. As the name suggests, molecules of this geometry have their atoms positioned at the corners. Examples Numerous compounds adopt this geometry, examples being especially numerous for transition metal complexes. The noble gas compound XeF4 adopts this structure as predicted by VSEPR theory. The geometry is prevalent for transition metal complexes with d8 configuration, which includes Rh(I), Ir(I), Pd(II), Pt(II), and Au(III). Notable examples include the anticancer drugs cisplatin [PtCl2(NH3)2] and carboplatin. Many homogeneous catalysts are square planar in their resting state, such as Wilkinson's catalyst and Crabtree's catalyst. Other examples include Vaska's complex and Zeise's salt. Certain ligands (such as porphyrins) stabilize this geometry. Splitting of d-orbitals Representative d-orbital splitting diagrams for square planar complexes featuring σ-donor (left) and σ+π-donor (right) ligands. A general d-orbital splitting diagram for square planar (D4h) transition metal complexes can be derived from the general octahedral (Oh) splitting diagram, in which the dz2 and the dx2−y2 orbitals are degenerate and higher in energy than the degenerate set of dxy, dxz and dyz orbitals. When the two axial ligands are removed to generate a square planar geometry, the dz2 orbital is driven lower in energy as electron-electron repulsion with ligands on the z-axis is no longer present. However, for purely σ-donating ligands the dz2 orbital is still higher in energy than the dxy, dxz and dyz orbitals because of the torus shaped lobe of the dz2 orbital. It bears electron density on the x- and y-axes and therefore interacts with the filled ligand orbitals. The dxy, dxz and dyz orbitals are generally presented as degenerate but they have to split into two different energy levels with respect to the irreducible representations of the point group D4h. Their relative ordering depends on the nature of the particular complex. Furthermore, the splitting of d-orbitals is perturbed by π-donating ligands in contrast to octahedral complexes. In the square planar case strongly π-donating ligands can cause the dxz and dyz orbitals to be higher in energy than the dz2 orbital, whereas in the octahedral case π-donating ligands only affect the magnitude of the d-orbital splitting and the relative ordering of the orbitals is conserved.[1] See also AXE method Molecular geometry References ^ Börgel, Jonas; Campbell, Michael G.; Ritter, Tobias (2016-01-12). "Transition Metal d-Orbital Splitting Diagrams: An Updated Educational Resource for Square Planar Transition Metal Complexes". Journal of Chemical Education. 93 (1): 118–121. Bibcode:2016JChEd..93..118B. doi:10.1021/acs.jchemed.5b00542. ISSN 0021-9584. External links 3D Chem – Chemistry, Structures, and 3D Molecules IUMSC – Indiana University Molecular Structure Center Interactive molecular examples for point groups [1] – Coordination numbers and complex ions Retrieved from " Molecular geometry Octahedral molecular geometryExamplesSF6, Mo(CO)6Point groupOhCoordination number6Bond angle(s)90°μ (Polarity)0 In chemistry, octahedral molecular geometry, also called square bipyramidal,[1] describes the shape of compounds with six atoms or groups of atoms or ligands symmetrically arranged around a central atom, defining the vertices of an octahedron. The octahedron has eight faces, hence the prefix octa. The octahedron is one of the Platonic solids, although octahedral molecules typically have an atom in their centre and no bonds between the ligand atoms. A perfect octahedron belongs to the point group Oh. Examples of octahedral compounds are sulfur hexafluoride SF6 and molybdenum hexacarbonyl Mo(CO)6. The term "octahedral" is used somewhat loosely by chemists, focusing on the geometry of the bonds to the central atom and not considering differences among the ligands themselves. For example, [Co(NH3)6]3+, which is not octahedral in the mathematical sense due to the orientation of the N−H bonds, is referred to as octahedral.[2] The concept of octahedral coordination geometry was developed by Alfred Werner to explain the stoichiometries and isomerism in coordination compounds. His insight allowed chemists to rationalize the number of isomers of coordination compounds. Octahedral transition-metal complexes containing amines and simple anions are often referred to as Werner-type complexes. Structure of sulfur hexafluoride, an example of a molecule with the octahedral coordination geometry. Isomerism in octahedral complexes Main article: Stereochemistry When two or more types of ligands (La, Lb, ...) are coordinated to an octahedral metal centre (M), the complex can exist as isomers. The naming system for these isomers depends upon the number and arrangement of different ligands. cis and trans For MLa4Lb2, two isomers exist. These isomers of MLa4Lb2 are cis, if the Lb ligands are mutually adjacent, and trans, if the Lb groups are situated 180° to each other. It was the analysis of such complexes that led Alfred Werner to the 1913 Nobel Prize–winning postulation of octahedral complexes. cis-[CoCl2(NH3)4]+ trans-[CoCl2(NH3)4]+ Facial and meridional isomers For MLa3Lb3, two isomers are possible - a facial isomer (fac) in which each set of three identical ligands occupies one face of the octahedron surrounding the metal atom, so that any two of these three ligands are mutually cis, and a meridional isomer (mer) in which each set of three identical ligands occupies a plane passing through the metal atom. fac-[CoCl3(NH3)3] mer-[CoCl3(NH3)3] Chirality More complicated complexes, with several different kinds of ligands or with bidentate ligands can also be chiral, with pairs of isomers which are non-superimposable mirror images or enantiomers of each other. Λ-[Fe(ox)3]3− Δ-[Fe(ox)3]3− Λ-cis-[CoCl2(en)2]+ Δ-cis-[CoCl2(en)2]+ Other For MLa2Lb2Lc2, a total of six isomers are possible.[3] One isomer in which all three pairs of identical ligands are trans Three distinct isomers in which one pair of identical ligands (La or Lb or Lc) is trans while the other two are cis. Two enantiomeric chiral isomers in which all three pairs of identical ligands are cis. The number of possible isomers can reach 30 for an octahedral complex with six different ligands (in contrast, only two stereoisomers are possible for a tetrahedral complex with four different ligands). The following table lists all possible combinations for monodentate ligands: Formula Number of isomers Number of enantiomeric pairs ML6 1 0 MLa5Lb 1 0 MLa4Lb2 2 0 MLa4LbLc 2 0 MLa3Lb3 2 0 MLa3Lb2Lc 3 0 MLa3LbLcLd 5 1 MLa2Lb2Lc2 6 1 MLa2Lb2LcLd 8 2 MLa2LbLcLdLe 15 6 MLaLbLcLdLeLf 30 15 Thus, all 15 diastereomers of MLaLbLcLdLeLf are chiral, whereas for MLa2LbLcLdLe, six diastereomers are chiral and three are not (the ones where La are trans). One can see that octahedral coordination allows much greater complexity than the tetrahedron that dominates organic chemistry. The tetrahedron MLaLbLcLd exists as a single enantiomeric pair. To generate two diastereomers in an organic compound, at least two carbon centers are required. Deviations from ideal symmetry Jahn–Teller effect Main article: Jahn–Teller effect The term can also refer to octahedral influenced by the Jahn–Teller effect, which is a common phenomenon encountered in coordination chemistry. This reduces the symmetry of the molecule from Oh to D4h and is known as a tetragonal distortion. Distorted octahedral geometry Some molecules, such as XeF6 or IF−6, have a lone pair that distorts the symmetry of the molecule from Oh to C3v.[4][5] The specific geometry is known as a monocapped octahedron, since it is derived from the octahedron by placing the lone pair over the centre of one triangular face of the octahedron as a "cap" (and shifting the positions of the other six atoms to accommodate it).[6] These both represent a divergence from the geometry predicted by VSEPR, which for AX6E1 predicts a pentagonal pyramidal shape. Bioctahedral structures Pairs of octahedra can be fused in a way that preserves the octahedral coordination geometry by replacing terminal ligands with bridging ligands. Two motifs for fusing octahedra are common: edge-sharing and face-sharing. Edge- and face-shared bioctahedra have the formulas [M2L8(μ-L)]2 and M2L6(μ-L)3, respectively. Polymeric versions of the same linking pattern give the stoichiometries [ML2(μ-L)2]∞ and [M(μ-L)3]∞, respectively. The sharing of an edge or a face of an octahedron gives a structure called bioctahedral. Many metal pentahalide and pentaalkoxide compounds exist in solution and the solid with bioctahedral structures. One example is niobium pentachloride. Metal tetrahalides often exist as polymers with edge-sharing octahedra. Zirconium tetrachloride is an example.[7] Compounds with face-sharing octahedral chains include MoBr3, RuBr3, and TlBr3. Ball-and-stick model of niobium pentachloride, a bioctahedral coordination compound. Ball-and-stick model of zirconium tetrachloride, an inorganic polymer based on edge-sharing octahedra. Ball-and-stick model of molybdenum(III) bromide, an inorganic polymer based on face-sharing octahedra. View almost down the chain of titanium(III) iodide highlighting the eclipsing of the halide ligands in such face-sharing octahedra. Trigonal prismatic geometry Main article: trigonal prismatic molecular geometry "Trigonal prism" redirects here. For the three-sided prism, see Triangular prism. For compounds with the formula MX6, the chief alternative to octahedral geometry is a trigonal prismatic geometry, which has symmetry D3h. In this geometry, the six ligands are also equivalent. There are also distorted trigonal prisms, with C3v symmetry; a prominent example is W(CH3)6. The interconversion of Δ- and Λ-complexes, which is usually slow, is proposed to proceed via a trigonal prismatic intermediate, a process called the "Bailar twist". An alternative pathway for the racemization of these same complexes is the Ray–Dutt twist. Splitting of d-orbital energies Main article: Ligand field theory For a free ion, e.g. gaseous Ni2+ or Mo0, the energy of the d-orbitals are equal in energy; that is, they are "degenerate". In an octahedral complex, this degeneracy is lifted. The energy of the dz2 and dx2−y2, the so-called eg set, which are aimed directly at the ligands are destabilized. On the other hand, the energy of the dxz, dxy, and dyz orbitals, the so-called t2g set, are stabilized. The labels t2g and eg refer to irreducible representations, which describe the symmetry properties of these orbitals. The energy gap separating these two sets is the basis of crystal field theory and the more comprehensive ligand field theory. The loss of degeneracy upon the formation of an octahedral complex from a free ion is called crystal field splitting or ligand field splitting. The energy gap is labeled Δo, which varies according to the number and nature of the ligands. If the symmetry of the complex is lower than octahedral, the eg and t2g levels can split further. For example, the t2g and eg sets split further in trans-MLa4Lb2. Ligand strength has the following order for these electron donors: weak: iodine < bromine < fluorine < acetate < oxalate < water < pyridine < cyanide :strong So called "weak field ligands" give rise to small Δo and absorb light at longer wavelengths. Reactions Given that a virtually uncountable variety of octahedral complexes exist, it is not surprising that a wide variety of reactions have been described. These reactions can be classified as follows: Ligand substitution reactions (via a variety of mechanisms) Ligand addition reactions, including among many, protonation Redox reactions (where electrons are gained or lost) Rearrangements where the relative stereochemistry of the ligand changes within the coordination sphere. Many reactions of octahedral transition metal complexes occur in water. When an anionic ligand replaces a coordinated water molecule the reaction is called an anation. The reverse reaction, water replacing an anionic ligand, is called aquation. For example, the [CoCl(NH3)5]2+ slowly yields [Co(NH3)5(H2O)]3+ in water, especially in the presence of acid or base. Addition of concentrated HCl converts the aquo complex back to the chloride, via an anation process. See also Octahedral clusters AXE method Molecular geometry References ^ "Trigonal bipyramidal molecular shape @ Chemistry Dictionary & Glossary". glossary.periodni.com. Retrieved 2022-07-03. ^ Von Zelewsky, A. (1995). Stereochemistry of Coordination Compounds. Chichester: John Wiley. ISBN 0-471-95599-X. ^ Miessler, G. L.; Tarr, D. A. (1999). Inorganic Chemistry (2nd ed.). Prentice-Hall. p. 290. ISBN 0-13-841891-8. ^ Crawford, T. Daniel; Springer, Kristen W.; Schaefer, Henry F. (1994). "A contribution to the understanding of the structure of xenon hexafluoride". J. Chem. Phys. 102 (8): 3307–3311. Bibcode:1995JChPh.102.3307C. doi:10.1063/1.468642. ^ Mahjoub, Ali R.; Seppelt, Konrad (1991). "The Structure of IF−6". 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