# Coordination geometries and benchmark data[1-4]

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **C.N.** | **Polyhedral symbol [5]** | **Name [4]** | **Coordination**  **polyhedron** | **Model** | **Angles (ideal)** | **Proteins, monuclear sites** | **Ideal coordinates** |
| 2 | L-2 | LIN | Linear[4, 5] |  | Planar | 171 |  |
|  | A-2 | TRV | Angular[5]  Trigonal plane with a vacancy[4] |  | Planar | 1859 |  |
| 3 | TP-3 | TRI | Trigonal plane[5] |  | Planar | 196 |  |
| 0 | TPY-3 | TEV | Trigonal pyramid[5]  Tetrahedron with a vacancy[4] |  |  | 963 |  |
| 3 | TS-3 | SPV | T-shape[5] Square plane with a vacancy[4] |  | Planar | 539 |  |
| 4 | T-4 | TET | Tetrahedron[4, 5] |  |  |  |  |
| 4 | SP-4 | SPL | Square plane[5] [4] |  | Planar |  |  |
| 4 | SPY-4 |  | Square pyramid[5] |  |  |  |  |
| 4 | SS-4 |  | See-saw[5] | [A] |  |  |  |
| 5 | TBPY-5 |  | Trigonal bipyramid |  |  |  |  |
| 5 | SPY-5 |  | Square pyramid |  |  |  |  |
| 6 | OC-6 |  | Octahedron |  |  |  |  |
| 6 | TPR-6 |  | Trigonal prism | [B] |  |  |  |
| 7 | PBPY-7 | PBP | pentagonal bipyramid |  |  |  |  |
| 7 | OCF-7 | COC | octahedron, face monocapped | [C] |  |  |  |
| 7 | TPRS-7 | CTP | trigonal prism, square-face monocapped | [D] |  |  |  |
| 7 |  | HVA | Hexagonal bipyramid with a vacancy (axial) |  |  |  |  |
| 7 |  | HVP | Hexagonal bipyramid with a vacancy (equatorial) |  |  |  |  |
| 7 |  | CUV | Cube with a vacancy |  |  |  |  |
| 7 |  | SAV | Square antiprism with a vacancy |  |  |  |  |
| 8 | CU-8 | CUB | cube |  |  |  |  |
| 8 | SAPR-8 | SQA | square antiprism | [E] |  |  |  |
| 8 | DD-8 |  | dodecahedron | [F] |  |  |  |
| 8 | HBPY-8 | HBP | hexagonal bipyramid |  |  |  |  |
| 8 | OCT-8 | BOC | octahedron, trans-bicapped |  |  |  |  |
| 8 | TPRT-8 | BTT | trigonal prism, triangular-face bicapped | [G] |  |  |  |
| 8 | TPRS-8 | BTS | trigonal prism, square-face bicapped | [H] |  |  |  |
| 9 | TPRS-9 | TTP | trigonal prism, square-face tricapped | [I] |  |  |  |
| 9 | HBPY-9 |  | heptagonal bipyramid | [J] |  |  |  |
| 9 |  | CSA | Square antiprism, square-face monocapped |  |  |  |  |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| [A] | [B] | [C] | [D] | [E] |
| [F] | [G] | [H] | [I] | [J] |

# Coordination Polyhedra - structural indices [6-12]

## for five-coordinated compounds [6]

Take the two largest valence angles in the compounds, such that ; indicates whether the structure is square pyramidal () , trigonal bipyramidal () or somewhere in between:

|  |  |  |  |
| --- | --- | --- | --- |
| Square pyramidal geometry | Square pyramidal geometry | Trigonal bipyramidal geometry | Trigonal bipyramidal geometry |

## for four-coordinated compounds [7, 8]

For four coordinate structures the parameter was developed. If the structure is square planar, then , while for tetrahedral structures :

Where and are like before, and

Unfortunately, the above formula does not distinguish and angles, so structures of significantly different geometries can have similar values. To overcome this issue, another structural index parameter was proposed[8], , that adopts values similar to but differentiated better the examined structures ():

In this expression are the two greatest valence angles of the coordination centre.

|  |  |  |
| --- | --- | --- |
| Square planar geometry | Seesaw geometry | Tetrahedral geometry |
| Square planar geometry | Seesaw geometry | Tetrahedral geometry |

## Proposal for for six-coordinated compounds

Limit complete geometries are octahedral and trigonal prismatic:

|  |  |  |  |
| --- | --- | --- | --- |
| **Octahedral geometry** | | **Trigonal prismatic** | |
|  |  | A picture containing accessory, umbrella  Description automatically generated | Regular triangular prism with 6xL atoms at the vertices and M atom at the centre of the prism. All M-L distances are defined to be of the same length. Angles are (see below for derivation): |

An example is trigonal prismatic , with a 9 ° deviation between the upper and lower pyramids, that displays a 80-84 angles and 130-140 angles.

|  |  |  |  |
| --- | --- | --- | --- |
| **Pentagonal bipyramid with a vacancy (axial)** | | **Pentagonal bipyramid with a vacancy (equatorial)** | |
|  | Angles: |  | Angles: |

Order should be Oct – vacEq – vacAx – TriPri ?

Or Oct – vacEq – TriPri – vacAx ?

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Octa | PBeqa | PBaxa | TriPa |  |
| d) | 180 | 180 | 144 | 135.585b) |  |
| d) | 180 | 144 | 144 | 135.585 |  |
| d) | 90 | 72 | 72 | 81.787c) |  |
| d) | 90 | 72 | 72 | 81.787 |  |
|  | 0 | 36 | 0 | 0 |  |
|  | 0 | 0 | 36 | 44.415 |  |
|  | 0 | 36 | 36 | 44.415 |  |
|  | div. by 0 | 0 | 1 | 1 |  |
|  | 180 | 144 | 180 | 180 |  |
|  | 0 | 0 | 0.25 | 0.327580485 |  |
|  | 0 | 0.25 | 0.25 | 0.327580485 |  |
|  | -0.3276 | -0.0621 | -0.2621 | -0.2468 |  |
|  | 90 | 108 | 72 | 53.798 |  |
|  | 90 | 72 | 72 | 53.798 |  |
|  | 1 | 1.5 | 1 | 0.6578 |  |
|  | 1 | 1 | 1 | 0.6578 |  |
|  | 0 | 0 | 0.2 | 0.24675 |  |
|  | 0 | 0.2 | 0.2 | 0.24675 |  |
|  | 0 | 0.2 | 0.4 | 0.4935 |  |
| e) f) | 0 | 0.4053 | 0.8105 | 1 |  |

**A)** Oct – octahedral coordination; PBEq - pentagonal bipyramid with equatorial vacancy; PBax - pentagonal bipyramid with axial vacancy; TriP – trigonal prismatic coordination; **B)** exact value is ; **C)** exact value is ; **D)** is the largest valence angle in the complex, and is the second largest; is the smallest angle, and is the second smallest; **E)** ; **F)** final form is:

### Angles in a regular triangular prism

Prism base is a regular triangle on the plane of side :

|  |  |
| --- | --- |
|  | from Pythagoras theorem  Red lines are the angle bisectors  D is the centre of the base:  Therefore,  D is the projection of the prism centre E on the base plan, therefore and |
|  | (ML bond length)  angle can be computed from dot product: |
|  | are the projections of on the plane (top of the prism); symmetrical to through  angles within each pyramid are equal  involving an L atom from each pyramid are: |

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