# Coordination geometries and benchmark data[1-4]

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| **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 |  |
| 2 | A-2 | TRV | Angular[5]  Trigonal plane with a vacancy[4] |  | Planar | 1859 |  |
| 3 | TP-3 | TRI | Trigonal plane[5] |  | Planar | 196 |  |
| 3 | 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)  [hexagonal pyramid] |  |  |  |  |
| 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 |  |  |  |  |

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