

Table S1. Idealized geometries included in the library of FindGeo (CN = coordination number, Name = three-letter code identifying the geometry in FindGeo, Description = description of the idealized geometry in terms of the corresponding ideal polyhedron or polygon, Symbol = polyhedral symbol denoting the geometry as taken from the “Red Book” (when present)).

| CN | Name | Description | Symbol |
|----|------|---|--------|
| 2 | lin | Linear | L-2 |
| | trv | Trigonal plane with a vacancy ^a | A-2 |
| 3 | tri | Trigonal plane | TP-3 |
| | tev | Tetrahedron with a vacancy ^b | TPY-3 |
| | spv | Square plane with a vacancy ^c | TS-3 |
| 4 | tet | Tetrahedron | T-4 |
| | spl | Square plane | SP-4 |
| | bva | Trigonal bipyramid with a vacancy (axial) | - |
| | bvp | Trigonal bipyramid with a vacancy (equatorial) ^d | SS-4 |
| | pyv | Square pyramid with a vacancy (equatorial) | - |
| 5 | spy | Square pyramid | SPY-5 |
| | tbp | Trigonal bipyramid | TBPY-5 |
| | tpv | Trigonal prism with a vacancy | - |
| 6 | oct | Octahedron | OC-6 |
| | tpr | Trigonal prism | TPR-6 |
| | pva | Pentagonal bipyramid with a vacancy (axial) | - |
| | pvp | Pentagonal bipyramid with a vacancy (equatorial) | - |
| | cof | Octahedron, face monocapped with a vacancy (capped face) | - |
| | con | Octahedron, face monocapped with a vacancy (non-capped face) | - |
| | ctf | Trigonal prism, square-face monocapped with a vacancy (capped face) | - |
| | ctn | Trigonal prism, square-face monocapped with a vacancy (non-capped edge) | - |
| 7 | pbp | Pentagonal bipyramid | PBPY-7 |
| | coc | Octahedron, face monocapped | OCF-7 |
| | ctp | Trigonal prism, square-face monocapped | TPRS-7 |
| | hva | Hexagonal bipyramid with a vacancy (axial) | - |
| | hvp | Hexagonal bipyramid with a vacancy (equatorial) | - |
| | cuv | Cube with a vacancy | - |
| | sav | Square antiprism with a vacancy | - |
| 8 | hbp | Hexagonal bipyramid | HBPY-8 |
| | cub | Cube | CU-8 |
| | sqa | Square antiprism | SAPR-8 |
| | boc | Octahedron, <i>trans</i> -bicapped | OCT-8 |
| | bts | Trigonal prism, square-face bicapped | TPRS-8 |
| | btt | Trigonal prism, triangular-face bicapped | TPRT-8 |
| 9 | ttp | Trigonal prism, square-face tricapped | TPRS-9 |
| | csa | Square antiprism, square-face monocapped | - |

^aAlso described as angular

^bAlso described as trigonal pyramid

^cAlso described as T-shape

^dAlso described as see-saw