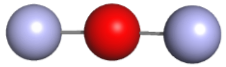
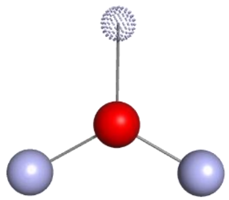
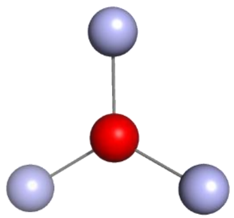
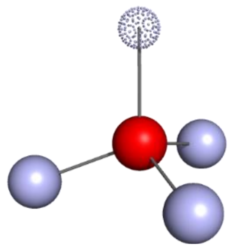
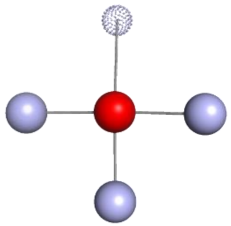
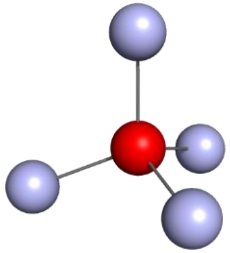
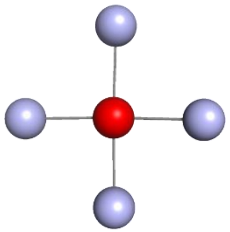
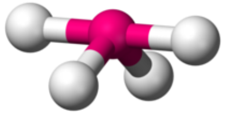
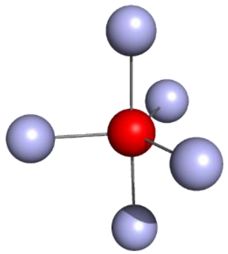
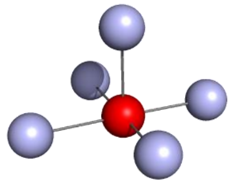
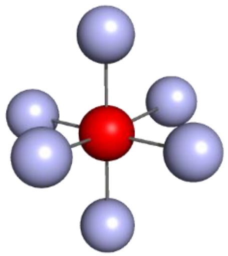
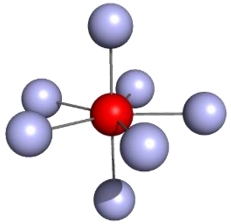
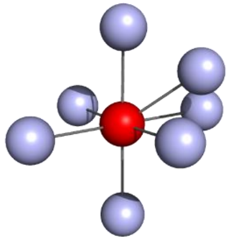
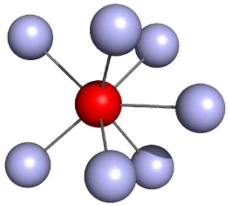
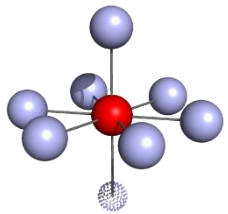
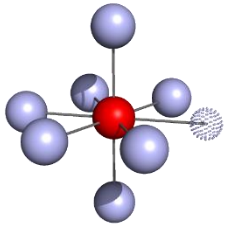
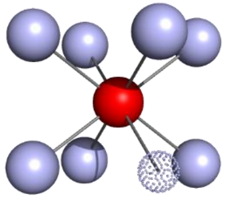
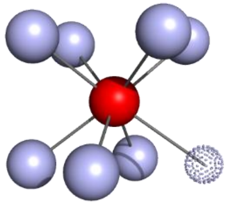
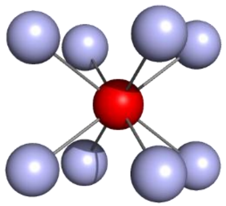
Coordination geometries and benchmark data[1-4]

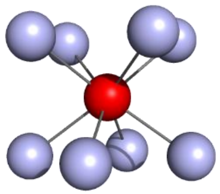
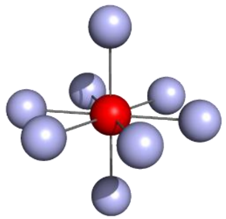
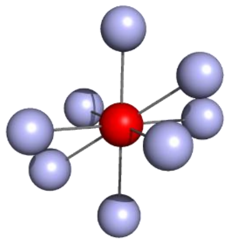
C.N.	Polyhedral symbol [5]	Name [4]	Coordination polyhedron	Model	Angles (ideal)	Proteins, monuclear sites	Ideal coordinates [Z]
2	L-2	LIN	Linear[4, 5]		Planar 180°	171	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & a & 0 & 0 \\ L_2 & -a & 0 & 0 \end{array}$
2	A-2	TRV	Angular[5] Trigonal plane with a vacancy[4]		Planar 120° 60°	1859	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & a & 0 & 0 \\ L_2 & -b & c & 0 \end{array}$
3	TP-3	TRI	Trigonal plane[5]		Planar 60°	196	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & c & -b & 0 \\ L_3 & -c & -b & 0 \end{array}$
3	TPY-3	TEV	Trigonal pyramid[5] Tetrahedron with a vacancy[4]		$L\widehat{M}L \approx 109.5°$ $\arccos\left(-\frac{1}{3}\right)$	963	Remove one (any) from tetrahedron

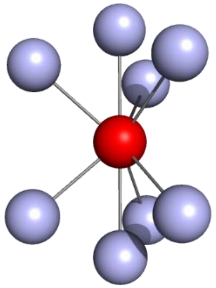
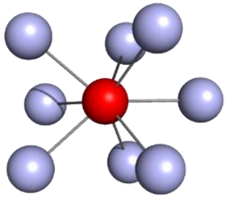
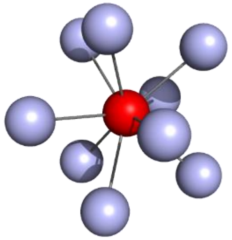
3	TS-3	SPV	T-shape[5] Square plane with a vacancy[4]		Planar 90° 180°	539	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & a & 0 & 0 \\ L_3 & 0 & -a & 0 \end{array}$
4	T-4	TET	Tetrahedron[4, 5]		$L\widehat{M}L = \arccos\left(-\frac{1}{3}\right)$ $\approx 109.4712°$		$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & d & 0 & -d \\ L_2 & -e & f & -d \\ L_3 & -e & -f & -d \\ L_4 & 0 & 0 & a \end{array}$
4	SP-4	SPL	Square plane[5] [4]		Planar 180° 90°		$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & a & 0 & 0 \\ L_3 & 0 & -a & 0 \\ L_4 & -a & 0 & 0 \end{array}$
4	SPY-4		Square pyramid[5]				$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & 0 & a & -a \\ L_2 & a & 0 & -a \\ L_3 & 0 & -a & -a \\ L_4 & -a & 0 & -a \end{array}$
4	SS-4		See-saw[5]	 [A]	$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 90°$		$\begin{array}{ccc} M & 0 & 0 \\ L_1 & 0 & a \\ L_2 & 0 & -a \\ L_3 & 0 & 0 \\ L_4 & a & 0 \\ L_6 & 0 & -a \end{array}$

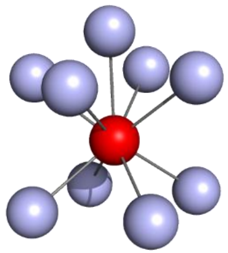
5	TBPY-5	Trigonal bipyramid		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 120°$	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & c & -b & 0 \\ L_3 & -c & -b & 0 \\ L_4 & 0 & 0 & a \\ L_5 & 0 & 0 & -a \end{array}$
5	SPY-5	Square pyramid		$L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 90°$	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & a & 0 & 0 \\ L_3 & 0 & -a & 0 \\ L_4 & -a & 0 & 0 \\ L_5 & 0 & 0 & a \end{array}$
6	OC-6	Octahedron		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq}$ $= 90°, 180°$	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & a & 0 & 0 \\ L_3 & 0 & -a & 0 \\ L_4 & -a & 0 & 0 \\ L_5 & 0 & 0 & a \\ L_6 & 0 & 0 & -a \end{array}$
6	TPR-6	Trigonal prism	[B]		$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & d & 0 & -d \\ L_2 & -e & f & -d \\ L_3 & -e & -f & -d \\ L_4 & d & 0 & d \\ L_5 & -e & f & d \\ L_6 & -e & -f & d \end{array}$

7	PBPY-7 [1/3 most frequente for CN 7]	PBP	pentagonal bipyramid		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 72°, 144°$	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & a & 0 & 0 \\ L_2 & i & j & 0 \\ L_3 & k & l & 0 \\ L_4 & k & -l & 0 \\ L_5 & i & -j & 0 \\ L_6 & 0 & 0 & a \\ L_7 & 0 & 0 & -a \end{array}$
7	OCF-7 [2/3 most frequente for CN 7]	COC	octahedron, face monocapped	 [C] [K]		
7	TPRS-7 [3/3 most frequente for CN 7]	CTP	trigonal prism, square-face monocapped	 [D] [L]		
7		HVA	Hexagonal bipyramid with a vacancy (axial) [hexagonal pyramid]		$L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 60°, 120°, 180°$	Remove L_8 or L_7 from hexagonal bipyramid

7		HVP	Hexagonal bipyramid with a vacancy (equatorial)		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq}$ $= 60°, 120°, 180°$	Remove one (any) from L_1 to L_6 from hexagonal bipyramid
7		CUV	Cube with a vacancy			Remove one (any) from cube
7		SAV	Square antiprism with a vacancy			Remove one (any) from square antiprism
8	CU-8	CUB	cube			$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & g & g & g \\ L_2 & -g & g & g \\ L_3 & g & -g & g \\ L_4 & g & g & -g \\ L_5 & -g & -g & g \\ L_6 & -g & g & -g \\ L_7 & g & -g & -g \\ L_8 & -g & -g & -g \end{array}$

8	SAPR-8	SQA	square antiprism	 [E]		$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & g & g & g \\ L_2 & -g & g & g \\ L_3 & g & -g & g \\ L_4 & a & 0 & -g \\ L_5 & -g & -g & g \\ L_6 & 0 & a & -g \\ L_7 & -a & 0 & -g \\ L_8 & 0 & -a & -g \end{array}$
8	DD-8		dodecahedron	[F] [M]		
8	HBPY-8	HBP	hexagonal bipyramid		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq}$ $= 60°, 120°, 180°$	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & a & 0 & 0 \\ L_2 & b & c & 0 \\ L_3 & -b & c & 0 \\ L_4 & -a & 0 & 0 \\ L_5 & -b & -c & 0 \\ L_6 & b & -c & 0 \\ L_7 & 0 & 0 & a \\ L_8 & 0 & 0 & -a \end{array}$
8	OCT-8	BOC	octahedron, trans-bicapped			

8	TPRT-8	BTT	trigonal prism, triangular-face bicapped	 [G] [N]
8	TPRS-8	BTS	trigonal prism, square-face bicapped	 [H]
9	TPRS-9	TTP **(similar to CSA)**	trigonal prism, square-face tricapped	 [I] [O]

9	HBPY-9		heptagonal bipyramid	[J]	$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = \left.\frac{360n}{7}\right\vert_{1\leq n\leq 4} \approx 51.428, 102.857, 154.286, 205.714°$	$\begin{array}{cccc} M & 0 & 0 & 0 \\ L_1 & a & 0 & 0 \\ L_2 & m & q & 0 \\ L_3 & n & r & 0 \\ L_4 & p & s & 0 \\ L_5 & p & -s & 0 \\ L_6 & n & -r & 0 \\ L_7 & m & -q & 0 \\ L_8 & 0 & 0 & a \\ L_9 & 0 & 0 & -a \end{array}$
9		CSA **(similar to TTP)**	Square antiprism, square-face monocapped [K] [P]			

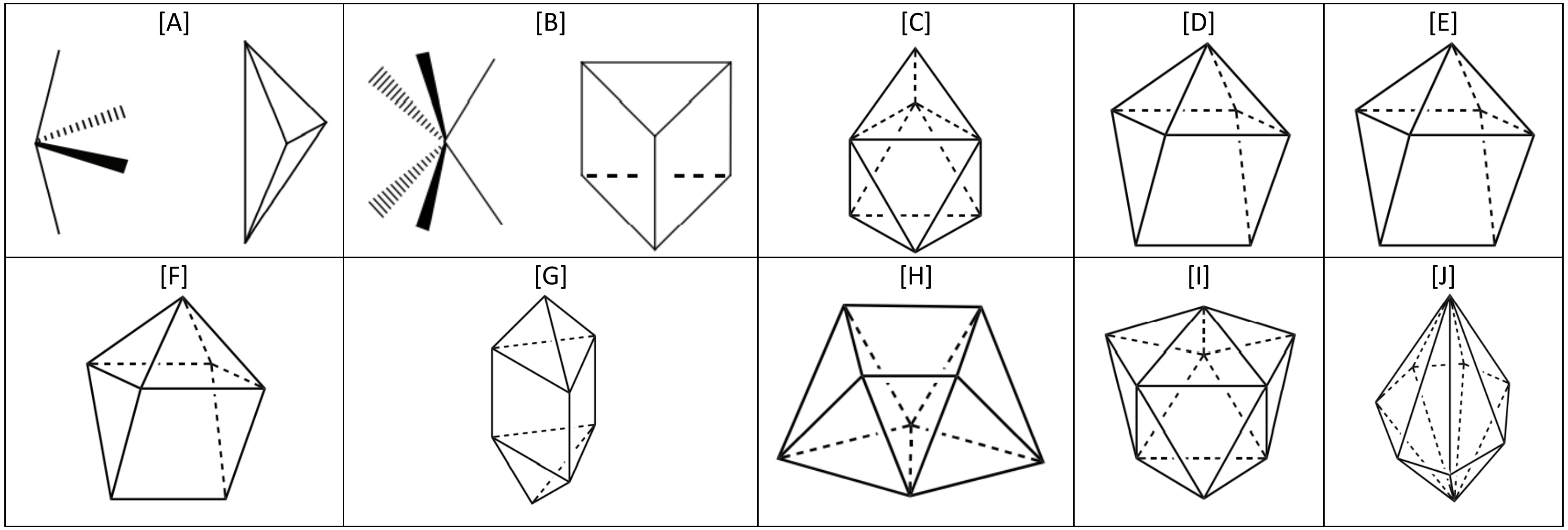
[Z]

$$b = \frac{a}{2} \qquad c = a\frac{\sqrt{3}}{2} \qquad d = a\frac{\sqrt{2}}{2} \qquad e = a\frac{\sqrt{2}}{4}$$

$$f = a\frac{\sqrt{6}}{4} \qquad g = a\frac{\sqrt{3}}{3} \qquad i = a\cos\left(\frac{2\pi}{5}\right) = \frac{a\left(\sqrt{5}-1\right)}{4} \qquad j = a\sin\left(\frac{2\pi}{5}\right) = \frac{a\sqrt{2\left(\sqrt{5}+5\right)}}{4}$$

$$k = a\cos\left(\frac{4\pi}{5}\right) = \frac{a\left(-\sqrt{5}-1\right)}{4} \qquad l = a\sin\left(\frac{4\pi}{5}\right) = \frac{a\sqrt{2\left(-\sqrt{5}+5\right)}}{4} \qquad m = a\cos\frac{2\pi}{7} \qquad n = a\cos\frac{4\pi}{7}$$

$$p = a\cos\frac{6\pi}{7} \qquad q = a\sin\frac{2\pi}{7} \qquad r = a\sin\frac{4\pi}{7} \qquad s = a\sin\frac{6\pi}{7}$$

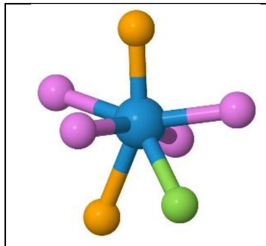

[A]
[B]
[C]
[D]
[E]
[F]
[G]
[H]
[I]
[J]

[K]

Capped octahedral molecular geometry, from the [gyroelongated triangular pyramid]

Ex.: CSD entry YIDBES

Deposition number 1302541 - WF_7^-

 Orange was axial Violet was equatorial Green is new	W2,5.117,1.893,2.108 F5,6.097,2.576,0.839 F6,4.739,1.217,3.889 F7,3.815,0.528,2.168 F8,3.78,2.198,0.923 F9,4.241,3.188,3.008 F10,6.569,2.669,3.134 F11,6.132,0.387,1.833

[L]

Capped trigonal prismatic, from augmented triangular prism (Johnson solid J49)

Ideal:

$$C \equiv O;\ edge = 2$$

$$\begin{array}{cccc} \pm 1 & -\frac{1}{\sqrt{3}} & \pm 1 & d = \frac{7}{3} \\ 0 & \frac{2}{\sqrt{3}} & \pm 1 & d = \frac{7}{3} \\ 0 & -\frac{1+\sqrt{6}}{\sqrt{3}} & 0 & d = \frac{2\sqrt{6}+7}{3} \end{array}$$

[M]

(Trigonal) Dodecahedron, from snub disphenoid (Johnson solid J84)

Ideal:

$$C \equiv O;\ edge = 2$$

$$\begin{array}{cccc} 0 & \sqrt{A} & \pm 1 & d = A+1 \\ \pm\sqrt{C} & \sqrt{B} & 0 & d = B+C \\ 0 & -\sqrt{B} & \pm\sqrt{C} & d = B+C \\ \pm 1 & -\sqrt{A} & 0 & d = A+1 \end{array}$$

$$A \in [2,3]: 2A^3 - A^2 - 8A - 4 = 0$$

$$B \in [0,1]: 2B^3 + 11B^2 + 4B - 1 = 0$$

$$C \in [1,2]: C^3 - 17C^2 + 64C - 64 = 0$$

$$\sqrt{A} = 1.567861848465127$$

$$\sqrt{B} = 0.411123131706519$$

$$\sqrt{C} = 1.289168546448310$$

[N]

Bicapped trigonal prismatic, from biaugmented triangular prism (Johnson solid J50)

Ideal:

$$C \equiv 0; edge = 2$$

$$\begin{array}{cccc} \pm 1 & -\frac{1}{\sqrt{3}} & \pm 1 & d = \frac{7}{3} \\ 0 & \frac{2}{\sqrt{3}} & \pm 1 & d = \frac{7}{3} \\ \pm\frac{1+\sqrt{6}}{2} & \frac{1+\sqrt{6}}{2\sqrt{3}} & 0 & d = \frac{(1+\sqrt{6})^2}{3} \end{array}$$

[O]

Tricapped trigonal prismatic, from triaugmented triangular prism (Johnson solid J51)

Ideal:

$$C \equiv 0; edge = 2$$

$$\begin{array}{cccc} \pm 1 & -\frac{1}{\sqrt{3}} & \pm 1 & d = \frac{7}{3} \\ 0 & \frac{2}{\sqrt{3}} & \pm 1 & d = \frac{7}{3} \\ \pm\frac{1+\sqrt{6}}{2} & \frac{1+\sqrt{6}}{2\sqrt{3}} & 0 & d = \frac{(1+\sqrt{6})^2}{3} \\ 0 & -\frac{1+\sqrt{6}}{\sqrt{3}} & 0 & d = \frac{(1+\sqrt{6})^2}{3} \end{array}$$

[P]

Capped square antiprismatic, from gyroelongated square pyramid (Johnson solid J10)

Ideal:

$$C \equiv 0; edge = 2$$

$$\begin{array}{cccc} 0 & 0 & \sqrt{2} + \frac{1}{\sqrt[4]{2}} & d = 2 + \frac{1}{\sqrt{2}} + 2\sqrt[4]{2} \\ 0 & \pm\sqrt{2} & \frac{1}{\sqrt[4]{2}} & d = 2 + \frac{1}{\sqrt{2}} \\ \pm\sqrt{2} & 0 & \frac{1}{\sqrt[4]{2}} & d = 2 + \frac{1}{\sqrt{2}} \\ \pm 1 & \pm 1 & -\frac{1}{\sqrt[4]{2}} & d = 2 + \frac{1}{\sqrt{2}} \end{array}$$