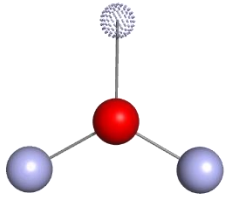
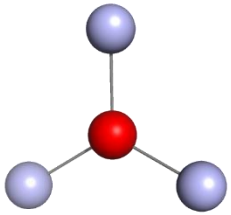
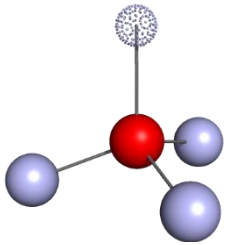
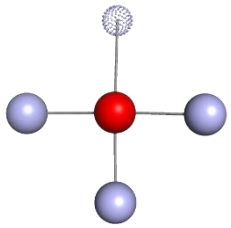
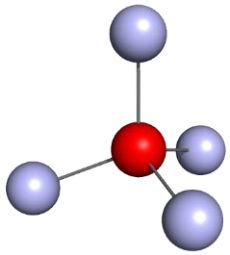
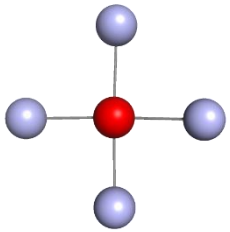
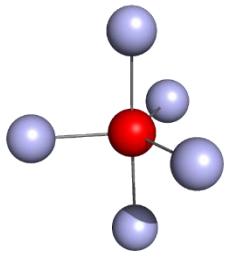
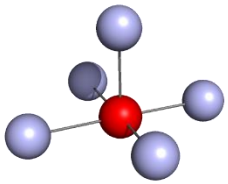
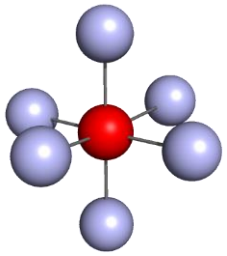
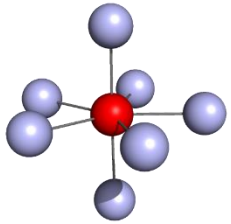
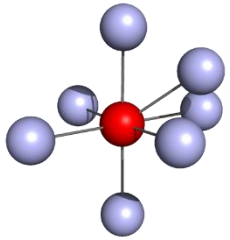
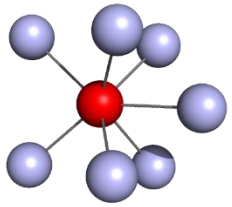
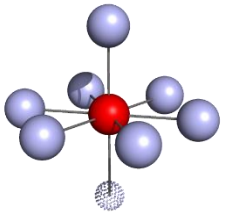
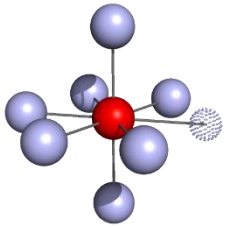
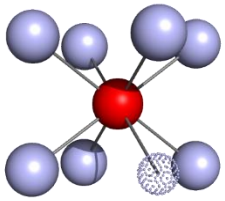
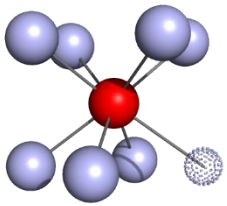
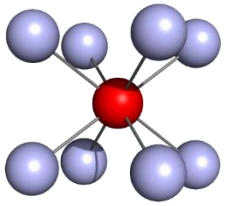
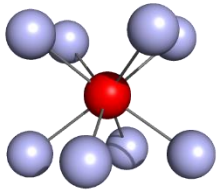
Coordination geometries and benchmark data[1-4]

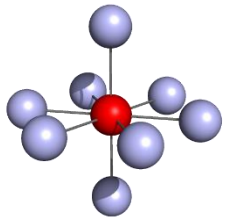
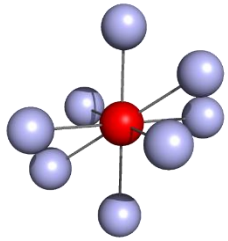
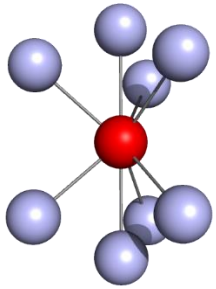
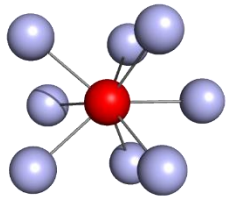
C.N.	Polyhedral symbol [5]	Name [4]	Coordination polyhedron	Model	Angles (ideal)	Proteins, monuclear sites	Ideal coordinates
2	L-2	LIN	Linear[4, 5]		Planar 180°	171	$M \quad 0 \quad 0 \quad 0$ $L_1 \quad a \quad 0 \quad 0$ $L_2 \quad -a \quad 0 \quad 0$
2	A-2	TRV	Angular[5] Trigonal plane with a vacancy[4]		Planar 120° 60°	1859	$M \quad 0 \quad 0 \quad 0$ $L_1 \quad a \quad 0 \quad 0$ $L_2 \quad -b \quad c \quad 0$ $\left(b = \frac{a}{2}; c = \frac{a\sqrt{3}}{2}\right)$
3	TP-3	TRI	Trigonal plane[5]		Planar 60°	196	$M \quad 0 \quad 0 \quad 0$ $L_1 \quad 0 \quad a \quad 0$ $L_2 \quad c \quad -b \quad 0$ $L_3 \quad -c \quad -b \quad 0$
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	

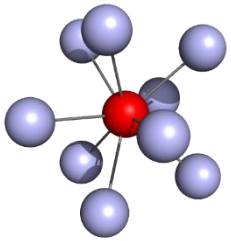
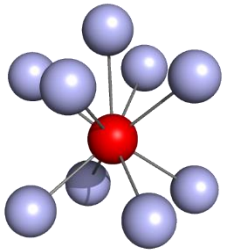
3	TS-3	SPV	T-shape[5] Square plane with a vacancy[4]		Planar 90° 180°	539	$\begin{matrix} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & a & 0 & 0 \\ L_3 & 0 & -a & 0 \end{matrix}$
4	T-4	TET	Tetrahedron[4, 5]		$L\widehat{M}L = \arccos\left(-\frac{1}{3}\right)$ $\approx 109.4712°$		
4	SP-4	SPL	Square plane[5]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

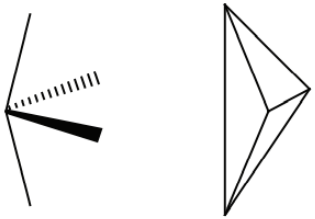
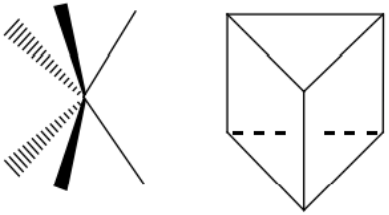
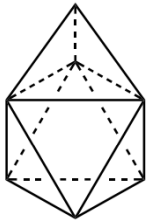
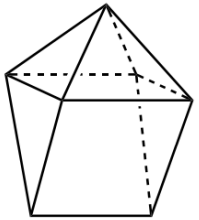
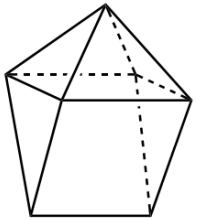
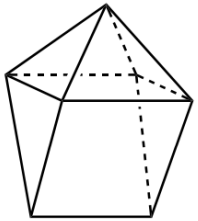
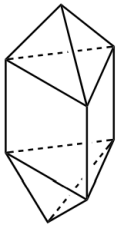
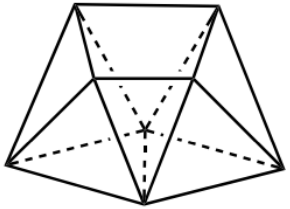
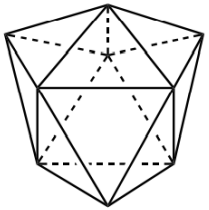
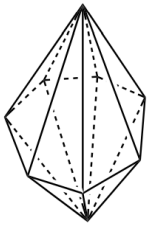
5	TBPY-5		Trigonal bipyramid		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 120°$	$\begin{matrix} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & c & -b & 0 \\ L_3 & -c & -b & 0 \\ L_4 & 0 & 0 & a \\ L_5 & 0 & 0 & -a \end{matrix}$
5	SPY-5		Square pyramid		$L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 90°$	$\begin{matrix} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & a & 0 & 0 \\ L_3 & 0 & -a & 0 \\ L_4 & -a & 0 & 0 \\ L_5 & 0 & 0 & a \end{matrix}$
6	OC-6		Octahedron		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 90°, 180°$	$\begin{matrix} M & 0 & 0 & 0 \\ L_1 & 0 & a & 0 \\ L_2 & a & 0 & 0 \\ L_3 & 0 & -a & 0 \\ L_4 & -a & 0 & 0 \\ L_5 & 0 & 0 & a \\ L_6 & 0 & 0 & -a \end{matrix}$
6	TPR-6		Trigonal prism	[B]		
7	PBPY-7	PBP	pentagonal bipyramid		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 72°, 144°$	

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]		$L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 60°, 120°, 180°$
7		HVP	Hexagonal bipyramid with a vacancy (equatorial)		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = 60°, 120°, 180°$

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		$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq}$ $= 60°, 120°, 180°$
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]	$L_{ax}\widehat{M}L_{ax} = 180°$ $L_{ax}\widehat{M}L_{eq} = 90°$ $L_{eq}\widehat{M}L_{eq} = \frac{360n}{7}\Big\vert_{1\leq n\leq 4} \approx 51.428, 102.857, 154.286, 205.714°$
9		CSA	Square antiprism, square-face monocapped		

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