

**Distortion Pathways of Transition Metal Coordination Polyhedra
Induced by Chelating Topology**

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Supporting Information

Coordinates for non-standard reference shapes (.ref file format for SHAPE 2.1)

fTPR-6

Flattened trigonal Prism

D3h

1.0000	0.0000	0.3464
-0.5000	0.8660	0.3464
-0.5000	-0.8660	0.3464
1.0000	0.0000	-0.3464
-0.5000	0.8660	-0.3464
-0.5000	-0.8660	-0.3464
0.0000	0.0000	0.0000

eTPR-6

Elongated trigonal Prism

D3h

1.0000000	0.0000000	-1.2990381
-0.5000000	0.8660254	-1.2990381
-0.5000000	-0.8660254	-1.2990381
1.0000000	0.0000000	1.2990381
-0.5000000	0.8660254	1.2990381
-0.5000000	-0.8660254	1.2990381
0.0000000	0.0000000	0.0000000

rect6

Rectangular equatorially distorted octahedron

C2v

1.00000	0.00000	0.00000
-1.00000	0.00000	0.00000
0.00000	1.00000	0.00000
0.00000	-1.00000	0.00000
0.00000	1.00000	0.00000
0.00000	-1.00000	0.00000
0.00000	0.00000	0.00000

Truncated Trigonal Pyramid

C3v

1.0000000	0.0000000	0.5000
-0.5000000	-0.8660000	0.5000
-0.5000000	0.8660000	0.5000
1.2500000	0.0000000	-0.5000
-0.6250000	-1.0825320	-0.5000
-0.6250000	1.0825320	-0.5000
0.0000000	0.0000000	-0.2810

ebcT-6

Edge bi-capped tetrahedron

D2d

0.0000000	0.81632653	-0.57723003
0.0000000	-0.81632653	-0.57723003

0.81632653	0.00000000	0.57723003
-0.81632653	0.00000000	0.57723003
0.00000000	0.00000000	1.00000000
0.00000000	0.00000000	-1.00000000
0.00000000	0.00000000	0.00000000

t6

2 doubled vertex tetrahedron

C2v

0.00000000	0.81632653	-0.57723003
0.00000000	-0.81632653	-0.57723003
0.81632653	0.00000000	0.57723003
-0.81632653	0.00000000	0.57723003
0.81632653	0.00000000	0.57723003
-0.81632653	0.00000000	0.57723003
0.00000000	0.00000000	0.00000000

vCOC-6

Vacant capped octahedron

C3v

0.0000	-0.9777	0.2101
0.8467	0.4888	0.2101
-0.8467	0.4888	0.2101
0.6284	-0.3628	-0.6881
-0.6284	-0.3628	-0.6881
0.0000	0.7257	-0.6881
0.0000	0.0000	0.0000

trapezoid6

Trapezoidal bipyramid

C2v

0.00000000	0.00000000	-1.00000000
1.00000000	0.00000000	0.00000000
1.00000000	0.00000000	0.00000000
-0.50000000	0.86602540	0.00000000
-0.50000000	-0.86602540	0.00000000
0.00000000	0.00000000	1.00000000
0.00000000	0.00000000	0.00000000

vPBPY-6

Equatorially-vacant Pentagonal Bipyramid

C2v

0.0000	0.0000	-1.0000
0.3090	0.9511	0.0000
-0.8090	0.5878	0.0000
-0.8090	-0.5878	0.0000
0.3090	-0.9511	0.0000
0.0000	0.0000	1.0000
0.0000	0.0000	0.0000

claw4
Closed pincer
Cinfv

0.00000	0.00000	1.00000
0.00000	0.00000	-1.00000
0.00000	0.00000	-1.00000
0.00000	0.00000	-1.00000
0.00000	0.00000	0.00000