

Supporting information

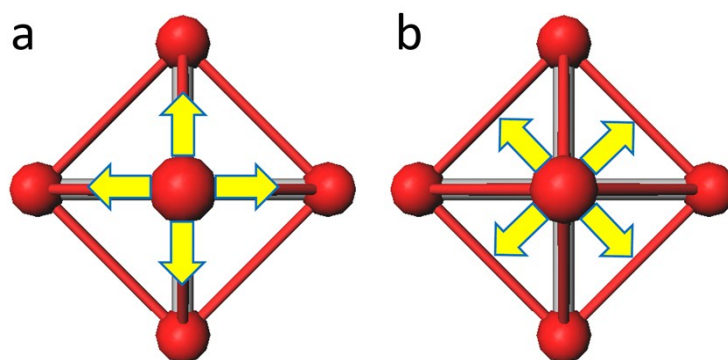


Figure S1. Edge directions (a) and bisecting directions (b) from an apex of an octahedron.

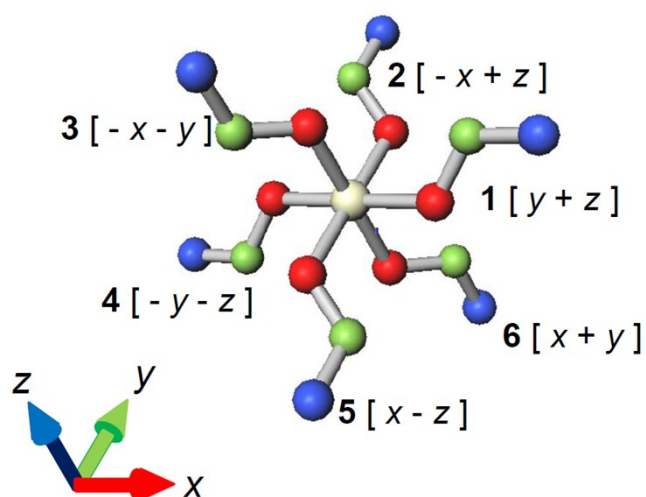


Figure S2. An example of a conformer with a numbering system.

Table S1. Bisected conformers of $[M(ABC)_6]$ possessing $M(AB)_6$ unit of S_6 symmetry^[a]

Code	Dihedral angles (°) of M-A-B-C units	Point Group
B3-1	[180, 180, 180, 180, 180, 180]	S_6
B3-2	[300, 60, 300, 60, 300, 60]	S_6
B3-3	[60, 300, 60, 300, 60, 300]	S_6
B3-4	[180, 60, 180, 60, 180, 60]	C_3
B3-5	[60, 180, 60, 180, 60, 180]	C_3
B3-6	[60, 60, 60, 60, 60, 60]	C_3
B3-7	[180, 300, 180, 180, 60, 180]	C_i
B3-8	[180, 300, 60, 180, 60, 300]	C_i
B3-9	[300, 180, 180, 60, 180, 180]	C_i
B3-10	[300, 180, 300, 60, 180, 60]	C_i
B3-11	[300, 180, 60, 60, 180, 300]	C_i
B3-12	[300, 300, 300, 60, 60, 60]	C_i
B3-13	[300, 300, 60, 60, 60, 300]	C_i
B3-14	[60, 180, 300, 300, 180, 60]	C_i
B3-15	[180, 180, 180, 180, 180, 300]	C_1
B3-16	[180, 180, 180, 180, 180, 60]	C_1
B3-17	[180, 180, 180, 180, 300, 300]	C_1
B3-18	[180, 180, 180, 180, 300, 60]	C_1
B3-19	[180, 180, 180, 180, 60, 300]	C_1
B3-20	[180, 180, 180, 180, 60, 60]	C_1
B3-21	[180, 180, 180, 300, 180, 300]	C_1

B3-22	[180, 180, 180, 300, 180, 60]	C_1
B3-23	[180, 180, 180, 300, 300, 300]	C_1
B3-24	[180, 180, 180, 300, 300, 60]	C_1
B3-25	[180, 180, 180, 300, 60, 300]	C_1
B3-26	[180, 180, 180, 300, 60, 60]	C_1
B3-27	[180, 180, 180, 60, 180, 300]	C_1
B3-28	[180, 180, 180, 60, 180, 60]	C_1
B3-29	[180, 180, 180, 60, 300, 300]	C_1
B3-30	[180, 180, 180, 60, 300, 60]	C_1
B3-31	[180, 180, 180, 60, 60, 300]	C_1
B3-32	[180, 180, 180, 60, 60, 60]	C_1
B3-33	[180, 180, 300, 180, 180, 300]	C_1
B3-34	[180, 180, 300, 180, 300, 300]	C_1
B3-35	[180, 180, 300, 180, 300, 60]	C_1
B3-36	[180, 180, 300, 180, 60, 300]	C_1
B3-37	[180, 180, 300, 180, 60, 60]	C_1
B3-38	[180, 180, 300, 300, 180, 300]	C_1
B3-39	[180, 180, 300, 300, 180, 60]	C_1
B3-40	[180, 180, 300, 300, 300, 300]	C_1
B3-41	[180, 180, 300, 300, 300, 60]	C_1
B3-42	[180, 180, 300, 300, 60, 300]	C_1
B3-43	[180, 180, 300, 300, 60, 60]	C_1
B3-44	[180, 180, 300, 60, 180, 300]	C_1
B3-45	[180, 180, 300, 60, 180, 60]	C_1
B3-46	[180, 180, 300, 60, 300, 300]	C_1

B3-47	[180, 180, 300, 60, 300, 60]	C_1
B3-48	[180, 180, 300, 60, 60, 300]	C_1
B3-49	[180, 180, 300, 60, 60, 60]	C_1
B3-50	[180, 180, 60, 180, 300, 300]	C_1
B3-51	[180, 180, 60, 180, 300, 60]	C_1
B3-52	[180, 180, 60, 180, 60, 300]	C_1
B3-53	[180, 180, 60, 180, 60, 60]	C_1
B3-54	[180, 180, 60, 300, 180, 300]	C_1
B3-55	[180, 180, 60, 300, 180, 60]	C_1
B3-56	[180, 180, 60, 300, 300, 300]	C_1
B3-57	[180, 180, 60, 300, 300, 60]	C_1
B3-58	[180, 180, 60, 300, 60, 300]	C_1
B3-59	[180, 180, 60, 300, 60, 60]	C_1
B3-60	[180, 180, 60, 60, 180, 300]	C_1
B3-61	[180, 180, 60, 60, 180, 60]	C_1
B3-62	[180, 180, 60, 60, 300, 300]	C_1
B3-63	[180, 180, 60, 60, 300, 60]	C_1
B3-64	[180, 180, 60, 60, 60, 300]	C_1
B3-65	[180, 180, 60, 60, 60, 60]	C_1
B3-66	[180, 300, 180, 300, 180, 60]	C_1
B3-67	[180, 300, 180, 300, 300, 300]	C_1
B3-68	[180, 300, 180, 300, 300, 60]	C_1
B3-69	[180, 300, 180, 300, 60, 300]	C_1
B3-70	[180, 300, 180, 300, 60, 60]	C_1
B3-71	[180, 300, 180, 60, 180, 60]	C_1

B3-72	[180, 300, 180, 60, 300, 300]	C_1
B3-73	[180, 300, 180, 60, 300, 60]	C_1
B3-74	[180, 300, 180, 60, 60, 300]	C_1
B3-75	[180, 300, 180, 60, 60, 60]	C_1
B3-76	[180, 300, 300, 180, 300, 300]	C_1
B3-77	[180, 300, 300, 180, 300, 60]	C_1
B3-78	[180, 300, 300, 180, 60, 300]	C_1
B3-79	[180, 300, 300, 300, 180, 60]	C_1
B3-80	[180, 300, 300, 300, 300, 300]	C_1
B3-81	[180, 300, 300, 300, 300, 60]	C_1
B3-82	[180, 300, 300, 300, 60, 300]	C_1
B3-83	[180, 300, 300, 300, 60, 60]	C_1
B3-84	[180, 300, 300, 60, 180, 60]	C_1
B3-85	[180, 300, 300, 60, 300, 300]	C_1
B3-86	[180, 300, 300, 60, 300, 60]	C_1
B3-87	[180, 300, 300, 60, 60, 300]	C_1
B3-88	[180, 300, 300, 60, 60, 60]	C_1
B3-89	[180, 300, 60, 180, 300, 300]	C_1
B3-90	[180, 300, 60, 180, 300, 60]	C_1
B3-91	[180, 300, 60, 300, 180, 60]	C_1
B3-92	[180, 300, 60, 300, 300, 300]	C_1
B3-93	[180, 300, 60, 300, 300, 60]	C_1
B3-94	[180, 300, 60, 300, 60, 300]	C_1
B3-95	[180, 300, 60, 300, 60, 60]	C_1
B3-96	[180, 300, 60, 60, 180, 60]	C_1

B3-97	[180, 300, 60, 60, 300, 300]	C_1
B3-98	[180, 300, 60, 60, 300, 60]	C_1
B3-99	[180, 300, 60, 60, 60, 300]	C_1
B3-100	[180, 300, 60, 60, 60, 60]	C_1
B3-101	[180, 60, 180, 60, 300, 300]	C_1
B3-102	[180, 60, 180, 60, 300, 60]	C_1
B3-103	[180, 60, 180, 60, 60, 300]	C_1
B3-104	[180, 60, 180, 60, 60, 60]	C_1
B3-105	[180, 60, 300, 180, 300, 300]	C_1
B3-106	[180, 60, 300, 300, 300, 300]	C_1
B3-107	[180, 60, 300, 300, 300, 60]	C_1
B3-108	[180, 60, 300, 300, 60, 300]	C_1
B3-109	[180, 60, 300, 300, 60, 60]	C_1
B3-110	[180, 60, 300, 60, 300, 300]	C_1
B3-111	[180, 60, 300, 60, 300, 60]	C_1
B3-112	[180, 60, 300, 60, 60, 300]	C_1
B3-113	[180, 60, 300, 60, 60, 60]	C_1
B3-114	[180, 60, 60, 300, 300, 300]	C_1
B3-115	[180, 60, 60, 300, 300, 60]	C_1
B3-116	[180, 60, 60, 300, 60, 300]	C_1
B3-117	[180, 60, 60, 300, 60, 60]	C_1
B3-118	[180, 60, 60, 60, 300, 300]	C_1
B3-119	[180, 60, 60, 60, 300, 60]	C_1
B3-120	[180, 60, 60, 60, 60, 300]	C_1
B3-121	[180, 60, 60, 60, 60, 60]	C_1

B3-122	[300, 300, 300, 300, 300, 60]	C_1
B3-123	[300, 300, 300, 300, 60, 300]	C_1
B3-124	[300, 300, 300, 300, 60, 60]	C_1
B3-125	[300, 300, 300, 60, 300, 60]	C_1
B3-126	[300, 300, 300, 60, 60, 300]	C_1
B3-127	[300, 300, 60, 300, 300, 60]	C_1
B3-128	[300, 300, 60, 300, 60, 300]	C_1
B3-129	[300, 300, 60, 300, 60, 60]	C_1
B3-130	[300, 300, 60, 60, 300, 60]	C_1

[a] The orientation is [$[y+z]$, $[-x+z]$, $[-x-y]$, $[-y-z]$, $[x-z]$, $[x+y]$].

Table S2. Resulting energies after structure optimization for $[\text{Mg}(\text{dmsO})_6]^{2+}$.

No	Code	Energy difference (kcal mol ⁻¹)
1	B3-3	0.00
2	B3-128	0.16
3	B3-13	0.39
4	B3-123	0.74
5	B3-129	0.85
6	B3-126	1.02
7	B3-130	1.18
8	B3-12	1.53
9	B3-127	1.59
10	B3-94	1.67

11	B3-125	1.72
12	B3-6	1.79
13	B3-124	1.83
14	B3-99	2.11
15	B3-92	2.27
16	B3-2	2.47
17	B3-80	2.49
18	B3-82	2.49
19	B3-116	2.55
20	B3-122	2.55
21	B3-118	2.58
22	B3-112	2.62
23	B3-110	2.79
24	B3-97	2.86
25	B3-98	3.01
26	B3-120	3.05
27	B3-85	3.08
28	B3-114	3.11
29	B3-100	3.12
30	B3-67	3.2
31	B3-86	3.23
32	B3-81	3.25
33	B3-72	3.26
34	B3-87	3.32
35	B3-108	3.52

36	B3-83	3.66
37	B3-93	3.67
38	B3-74	3.69
39	B3-69	3.7
40	B3-95	3.89
41	B3-121	3.9
42	B3-14	3.91
43	B3-106	3.95
44	B3-117	3.97
45	B3-88	3.98
46	B3-109	4.03
47	B3-78	4.05
48	B3-103	4.23
49	B3-115	4.28
50	B3-58	4.43
51	B3-59	4.52
52	B3-101	4.52
53	B3-8	4.54
54	B3-79	4.65
55	B3-73	4.67
56	B3-111	4.76
57	B3-84	4.79
58	B3-89	4.91
59	B3-113	4.92
60	B3-75	4.93

61	B3-40	5.01
62	B3-76	5.03
63	B3-64	5.07
64	B3-107	5.11
65	B3-119	5.11
66	B3-56	5.23
67	B3-91	5.28
68	B3-96	5.48
69	B3-70	5.52
70	B3-47	5.54
71	B3-41	5.59
72	B3-68	5.61
73	B3-5	5.66
74	B3-42	5.72
75	B3-43	5.73
76	B3-102	5.73
77	B3-63	5.77
78	B3-65	5.77
79	B3-60	5.88
80	B3-50	5.9
81	B3-104	6
82	B3-90	6.05
83	B3-49	6.17
84	B3-53	6.27
85	B3-57	6.32

86	B3-38	6.36
87	B3-77	6.44
88	B3-62	6.46
89	B3-39	6.48
90	B3-48	6.48
91	B3-23	6.66
92	B3-31	6.67
93	B3-46	6.67
94	B3-71	6.85
95	B3-25	6.87
96	B3-105	6.91
97	B3-66	6.96
98	B3-34	7
99	B3-54	7.18
100	B3-45	7.19
101	B3-52	7.19
102	B3-11	7.2
103	B3-26	7.22
104	B3-32	7.45
105	B3-10	7.74
106	B3-30	7.82
107	B3-35	8
108	B3-4	8.18
109	B3-55	8.29
110	B3-37	8.3

111	B3-51	8.37
112	B3-36	8.51
113	B3-29	8.73
114	B3-24	8.78
115	B3-17	8.83
116	B3-44	8.87
117	B3-61	9.05
118	B3-22	9.06
119	B3-9	9.32
120	B3-21	9.41
121	B3-27	9.5
122	B3-28	9.58
123	B3-20	9.72
124	B3-7	9.98
125	B3-19	10.01
126	B3-33	11.35
127	B3-18	11.99
128	B3-16	12.17
129	B3-15	12.69
130	B3-1	16.25
