Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

for

"Structure determination of neutral MgO clusters – hexagonal nanotubes and cages"

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Calculated vertical ionization energies:

# of MgO units	Vertical ionization energy (in eV)
1	8.72
2	7.71
3	8.49
4	8.27(T_d), 8.19(D_{4h}), 6.12(C_1)
5	7.56
6	7.87
7	8.04
8	7.85
9	7.94
10	7.62
11	7.64(C_s), 7.64(C_1)
12	7.75(D_{3d}), 7.89(T_h)
13	7.27(C_1), 7.25(C_3A), 7.28(C_3B)
14	7.54(C_1A), 7.6(C_1B), 7.47(C_1C)
15	7.70(D_{3h}), 7.73(C_{3h})
16	7.33(C_2), 7.60(C_{3v})

Lowest energy structures for $(MgO)_{15}$ with a cubic sub-structure:

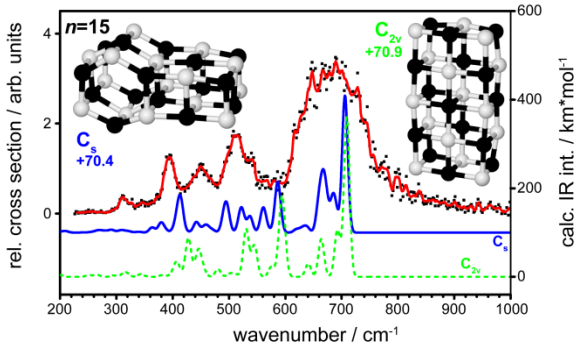

Figure S1: Comparison of the IR-UV two-color ionization spectrum of $(MgO)_{15}$ with the predicted linear absorption spectra for structures containing a cubic motif.

XYZ coordinates of all the structures shown in the article (in Å):

$(MgO)_3$:

D_{3h}

Mg	0.844605	1.462898	0.000000
Mg	0.844605	-1.462898	0.000000
Mg	-1.689209	0.000000	0.000000
O	-0.972076	1.683685	0.000000
O	1.944152	0.000000	0.000000
O	-0.972076	-1.683685	0.000000

$(MgO)_4$:

T_d

Mg	0.927890	-0.927890	0.927890
Mg	-0.927890	0.927890	0.927890
Mg	-0.927890	-0.927890	-0.927890
Mg	0.927890	0.927890	-0.927890
O	1.021977	-1.021977	-1.021977
O	-1.021977	-1.021977	1.021977
O	-1.021977	1.021977	-1.021977
O	1.021977	1.021977	1.021977

D_{4h}

Mg	1.5751013	1.5751013	0.0000000
Mg	-1.5751013	-1.5751013	0.0000000
Mg	1.5751013	-1.5751013	0.0000000
Mg	-1.5751013	1.5751013	0.0000000
O	2.4790119	0.0000000	0.0000000
O	0.0000000	-2.4790119	0.0000000
O	-2.4790119	0.0000000	0.0000000
O	0.0000000	2.4790119	0.0000000

C_1

O	-1.3150372	0.6062777	0.0681791
Mg	-0.5900141	-1.1810226	-0.3771907
O	1.2025330	-0.5674999	-0.0994474
Mg	3.0326109	-0.2436125	0.1025470
Mg	0.4869771	1.1712207	0.3335458
Mg	-3.1390359	0.6901452	-0.0167786
O	-4.8893364	1.2941353	-0.6695019
O	-4.9521076	1.0291974	0.6586466

$(MgO)_5$:

C_s

Mg	-2.344101	0.843740	0.000000
Mg	0.640705	0.933597	1.283272
Mg	-0.771221	-1.472817	0.000000
Mg	0.640705	0.933597	-1.283272
Mg	1.890277	-0.946241	0.000000
O	-0.681170	1.676889	0.000000
O	0.547305	-0.998025	1.406497
O	2.101427	0.966818	0.000000
O	-2.571194	-0.939521	0.000000
O	0.547305	-0.998025	-1.406497

$(MgO)_6$:

D_{3d}

Mg	1.594443	0.920552	0.950521
Mg	-1.594443	-0.920552	-0.950521

Mg	1.594443	-0.920552	-0.950521
Mg	0.000000	1.841104	-0.950521
Mg	-1.594443	0.920552	0.950521
Mg	0.000000	-1.841104	0.950521
O	-1.701223	0.982202	-1.045281
O	1.701223	0.982202	-1.045281
O	0.000000	-1.964403	-1.045281
O	1.701223	-0.982202	1.045281
O	0.000000	1.964403	1.045281
O	-1.701223	-0.982202	1.045281

$(MgO)_7$:

C_{3v}

Mg	0.000000	0.000000	2.888326
Mg	0.885350	-1.533471	0.942549
Mg	-0.749557	1.298270	-1.835630
Mg	0.885350	1.533471	0.942549
Mg	1.499113	0.000000	-1.835630
Mg	-1.770700	0.000000	0.942549
Mg	-0.749557	-1.298270	-1.835630
O	1.649813	0.000000	1.887274
O	-0.824907	-1.428780	1.887274
O	0.950292	1.645955	-0.939406
O	0.000000	0.000000	-3.053114
O	-1.900585	0.000000	-0.939406
O	0.950292	-1.645955	-0.939406
O	-0.824907	1.428780	1.887274

$(MgO)_8$:

S_4

Mg	1.363775	-1.402027	0.776576
Mg	-1.402027	-1.363775	-0.776576
Mg	-0.669924	-1.120980	2.455135
Mg	0.669924	1.120980	2.455135
Mg	1.402027	1.363775	-0.776576
Mg	1.120980	-0.669924	-2.455135
Mg	-1.120980	0.669924	-2.455135
Mg	-1.363775	1.402027	0.776576
O	-0.525318	-2.014018	0.768453
O	-0.691205	-1.251994	-2.556835
O	1.251994	-0.691205	2.556835
O	0.525318	2.014018	0.768453
O	-1.251994	0.691205	2.556835
O	-2.014018	0.525318	-0.768453
O	0.691205	1.251994	-2.556835
O	2.014018	-0.525318	-0.768453

$(MgO)_9$:

D_{3h}

Mg	1.822630	0.000000	1.928959
Mg	1.822630	0.000000	-1.928959
Mg	1.017278	1.761977	0.000000
Mg	-0.911315	1.578444	-1.928959
Mg	1.017278	-1.761977	0.000000
Mg	-0.911315	1.578444	1.928959
Mg	-2.034555	0.000000	0.000000
Mg	-0.911315	-1.578444	-1.928959
Mg	-0.911315	-1.578444	1.928959
O	0.986567	-1.708784	-2.006668
O	-1.044544	1.809204	0.000000
O	0.986567	-1.708784	2.006668
O	2.089088	0.000000	0.000000
O	0.986567	1.708784	2.006668
O	0.986567	1.708784	-2.006668
O	-1.973134	0.000000	2.006668
O	-1.973134	0.000000	-2.006668
O	-1.044544	-1.809204	0.000000

$(MgO)_{10}$:

C_2

Mg	0.927043	2.000815	0.912227
Mg	2.235206	-0.940373	1.731315
Mg	3.240052	0.905961	0.174257
Mg	1.929137	-1.798974	-0.742825
Mg	-0.927043	-2.000815	0.912227
Mg	-0.930288	-0.947060	-2.065723
Mg	-1.929137	1.798974	-0.742825
Mg	-3.240052	-0.905961	0.174257
Mg	-2.235206	0.940373	1.731315
Mg	0.930288	0.947060	-2.065723
O	0.946596	-2.114631	0.939346
O	-2.225221	-0.963576	1.872232
O	0.991652	-1.000885	-2.173193
O	-0.991652	1.000885	-2.173193
O	-1.935720	-1.915329	-0.789454
O	-3.413946	0.974385	0.141818
O	2.225221	0.963576	1.872232
O	3.413946	-0.974385	0.141818
O	-0.946596	2.114631	0.939346
O	1.935720	1.915329	-0.789454

$(MgO)_{11}$:

C_s

Mg	-1.4789607	1.6687347	1.6168682
Mg	0.6065093	1.2045839	-3.1287557
Mg	1.2880032	1.9814197	0.0000000
Mg	-1.4789607	1.6687347	-1.6168682
Mg	-0.1570368	-2.7018623	0.0000000
Mg	2.0895248	-0.9310870	1.3320706
Mg	-2.1478149	-0.9675373	0.0000000
Mg	-0.6658651	-1.0837934	-2.9005370
Mg	2.0895248	-0.9310870	-1.3320706
Mg	0.6065093	1.2045839	3.1287557
Mg	-0.6658651	-1.0837934	2.9005370
O	1.6832269	-2.2853671	0.0000000
O	-1.2749940	0.6972372	-3.2502133
O	0.3540092	2.3477915	-1.6234956
O	0.3540092	2.3477915	1.6234956
O	1.2400573	-0.6003522	-2.9841429
O	-1.3042306	-2.0134356	-1.3975672
O	-2.2208595	0.9596600	0.0000000
O	2.4220755	0.4341069	0.0000000
O	-1.3042306	-2.0134356	1.3975672
O	-1.2749940	0.6972372	3.2502133
O	1.2400573	-0.6003522	2.9841429

C_1

Mg	3.2038504	-0.0058789	-0.9017562
Mg	2.0754186	-1.1831893	1.7565225
Mg	-0.5029887	-1.6008612	1.0788278
Mg	1.1970773	-2.4639229	-0.9270515

Mg	0.5578115	0.0802507	-1.8351270
Mg	1.9105800	1.4146475	1.0022569
Mg	0.5102656	2.6954992	-0.8854900
Mg	-2.4136913	1.3262610	-0.9758669
Mg	-0.7247718	1.6006363	1.6876339
Mg	-3.4085306	-0.1991033	0.9453282
Mg	-2.3885397	-1.6946084	-0.9112109
O	1.9534482	1.4473704	-1.0367236
O	0.5695214	2.8320554	1.0203008
O	0.4838639	0.0366686	1.8139292
O	2.1757324	-1.2093739	-1.9272909
O	-0.5029042	-1.5265724	-1.1169522
O	1.1815699	-2.6451743	0.9704515
O	3.3173443	0.0368674	1.0246730
O	-0.7504764	1.6191017	-1.8184635
O	-2.4754051	1.4599945	1.0081046
O	-2.4101896	-1.8132344	1.0480623
O	-3.5589870	-0.2074325	-1.0201580

$(MgO)_{12}$:

D_{3d}

Mg	-1.7445893	1.0072391	-0.9862332
Mg	-1.5817767	-0.9132392	-2.9095876
Mg	-1.7445893	-1.0072391	0.9862332
Mg	1.7445893	-1.0072391	0.9862332
Mg	0.0000000	-1.8264784	2.9095876
Mg	1.5817767	0.9132392	2.9095876
Mg	-1.5817767	0.9132392	2.9095876
Mg	0.0000000	2.0144782	0.9862332
Mg	1.7445893	1.0072391	-0.9862332
Mg	0.0000000	1.8264784	-2.9095876
Mg	1.5817767	-0.9132392	-2.9095876
Mg	0.0000000	-2.0144782	-0.9862332
O	1.7037985	-0.9836885	2.9890318
O	-1.7037985	-0.9836885	2.9890318
O	1.8078650	1.0437713	0.9725426
O	0.0000000	1.9673771	2.9890318
O	-1.8078650	1.0437713	0.9725426
O	0.0000000	2.0875427	-0.9725426
O	1.8078650	-1.0437713	-0.9725426
O	-1.8078650	-1.0437713	-0.9725426
O	1.7037985	0.9836885	-2.9890318
O	-1.7037985	0.9836885	-2.9890318
O	0.0000000	-2.0875427	0.9725426
O	0.0000000	-1.9673771	-2.9890318

T_h

Mg	0.0000000	-1.3288854	2.6437183
Mg	-2.6437183	0.0000000	1.3288854
Mg	0.0000000	1.3288854	2.6437183
Mg	-2.6437183	0.0000000	-1.3288854
Mg	-1.3288854	-2.6437183	0.0000000
Mg	0.0000000	-1.3288854	-2.6437183
Mg	1.3288854	-2.6437183	0.0000000
Mg	1.3288854	2.6437183	0.0000000
Mg	2.6437183	0.0000000	1.3288854
Mg	-1.3288854	2.6437183	0.0000000
Mg	0.0000000	1.3288854	-2.6437183
Mg	2.6437183	0.0000000	-1.3288854
O	-2.7469442	-1.4075082	0.0000000
O	0.0000000	-2.7469442	1.4075082
O	1.4075082	0.0000000	2.7469442
O	-1.4075082	0.0000000	2.7469442
O	-2.7469442	1.4075082	0.0000000
O	0.0000000	-2.7469442	-1.4075082
O	2.7469442	1.4075082	0.0000000
O	0.0000000	2.7469442	1.4075082
O	0.0000000	2.7469442	-1.4075082
O	2.7469442	-1.4075082	0.0000000
O	-1.4075082	0.0000000	-2.7469442
O	1.4075082	0.0000000	-2.7469442

C_s

O	0.1639738	3.9423417	-1.9707894
Mg	1.9647566	3.3033650	-1.9041625
Mg	0.1056115	3.9586519	-0.0000024
O	2.2449679	3.3564370	-0.0000112
O	0.1639901	3.9423480	1.9707862
Mg	1.9647691	3.3033622	1.9041406
Mg	-0.4048272	2.0549000	2.0201494
O	1.5890977	1.4128129	2.0671646
O	-0.5446456	2.0628202	0.0000006
Mg	1.6142401	1.3963983	-0.0000212
Mg	-0.4048382	2.0548889	-2.0201443
O	1.5891039	1.4128096	-2.0671720
O	-1.0369236	0.1771017	-2.1617045
Mg	0.9333934	-0.4587614	-2.0675123
Mg	-1.0412922	0.1877861	0.0000582
O	0.9080266	-0.4441597	0.0000133
O	-1.0369507	0.1770949	2.1617241
Mg	0.9333985	-0.4587579	2.0675295
Mg	-0.1662479	-3.5809043	-1.9354769
O	1.2728546	-2.3577937	-2.0160355
O	-0.1216631	-3.8587744	-0.0000072
Mg	1.3037752	-2.3854726	0.0000102
Mg	-0.1662690	-3.5809161	1.9354619
O	1.2728292	-2.3577943	2.0160571
O	-2.0265922	-3.1566935	2.0065569
Mg	-2.2588737	-1.2801207	1.9507770
O	-2.4767736	-1.1811678	-0.0000033
Mg	-2.0534724	-3.2050261	-0.0000199
O	-2.0265687	-3.1566844	-2.0065777
Mg	-2.2588502	-1.2800916	-1.9507895

C_{2v}

Mg	-3.8719786	1.9064282	0.8848560
O	-3.9437551	1.9691193	-1.0223328
O	-4.0074664	-0.0000006	1.1500645
Mg	-3.9410750	-0.0000002	-1.0762751
Mg	-3.8719781	-1.9064289	0.8848557
O	-3.9437547	-1.9691195	-1.0223331
O	-1.9604634	-2.0857963	1.1089593
Mg	-1.9685792	-2.0213978	-1.0165439
Mg	-1.9570064	0.0000008	1.1497445
O	-1.9406496	0.0000005	-1.1005007
O	-1.9604637	2.0857967	1.1089600
Mg	-1.9685792	2.0213981	-1.0165437
Mg	-0.0000003	2.0432532	0.9963092
O	-0.0000001	2.1134839	-1.0612146
O	-0.0000000	0.0000000	1.1562607
Mg	0.0000006	-0.0000010	-1.0922845
Mg	-0.0000003	-2.0432529	0.9963092
O	0.0000000	-2.1134836	-1.0612151

O	1.9604633	-2.0857961	1.1089594
Mg	1.9685792	-2.0213981	-1.0165437
Mg	1.9570064	0.0000010	1.1497445
O	1.9406501	0.0000002	-1.1005010
O	1.9604635	2.0857969	1.1089596
Mg	1.9685792	2.0213981	-1.0165438
Mg	3.8719780	-1.9064288	0.8848560
O	3.9437548	-1.9691198	-1.0223327
O	4.0074664	-0.0000005	1.1500644
Mg	3.9410753	-0.0000005	-1.0762752
Mg	3.8719785	1.9064283	0.8848556
O	3.9437549	1.9691192	-1.0223331

$(MgO)_{13}$:

C_1

Mg	-3.2318845	-0.7463103	1.8169346
Mg	-1.5902138	1.0251201	-2.2370895
Mg	-0.4475744	0.8749110	2.0271005
Mg	-3.2565798	1.5124503	0.4768156
Mg	-3.0458750	-1.3849117	-0.7136632
Mg	-0.4160282	2.6691796	-0.5827801
Mg	4.0238907	0.1540024	0.2889076
Mg	-0.1243082	-1.7137363	-2.0585064
Mg	2.1844917	-2.1660617	-0.8511248
Mg	2.3269293	-0.8414099	2.0125223
Mg	-0.4752905	-2.2433812	1.0194047
Mg	2.3149543	2.0427659	0.8919052
Mg	1.8376950	0.8297112	-2.0744336
O	-1.8434078	-0.8738646	-2.1266275
O	-2.3474738	0.9239126	2.1140515
O	-2.2607830	2.2742141	-0.9147984
O	-2.3609309	-2.1835509	0.9351844
O	-4.1752673	-0.1439965	0.2183488
O	1.6643395	-1.0535007	-2.3482733
O	0.1843557	1.7620390	-2.1740366
O	0.4055023	-2.8102404	-0.5596563
O	3.3460605	-1.6193767	0.5223368
O	0.4518522	2.3163360	1.0686768
O	0.4256657	-0.8712473	2.0680142
O	3.2886432	0.8135968	1.9719553
O	3.1212363	1.4533491	-0.7911657

C_3A

Mg	-1.2573231	1.1574907	-1.0423377
Mg	1.6310779	0.5101284	-1.0423377
Mg	0.0000000	0.0000000	-3.1628898
Mg	2.2442052	-2.1277104	-0.8968539
Mg	-2.5177025	2.0403966	1.0781041
Mg	-1.4249892	-0.7490317	1.7398110
Mg	0.7205487	3.0073939	-0.8968539
Mg	-2.9647539	-0.8796835	-0.8968539
Mg	-0.3737548	-1.6676191	-1.0423377
Mg	-0.5081840	-3.2005926	1.0781041
Mg	3.0258865	1.1601961	1.0781041
Mg	1.3611751	-0.8595610	1.7398110
Mg	0.0638141	1.6085927	1.7398110
O	-1.5748420	-0.6245507	-2.2540421
O	1.3282978	-1.0515778	-2.2540421
O	0.2465442	1.6761285	-2.2540421
O	2.8135966	-0.6817862	0.2718121
O	-1.6851718	1.0344193	2.4236182
O	-3.1009183	0.9246707	-0.3379559
O	-1.9972425	-2.0957530	0.2718121
O	-0.8163541	2.7775392	0.2718121
O	0.0000000	0.0000000	0.2164222
O	2.3512475	2.2231387	-0.3379559
O	1.7384193	0.9421919	2.4236182
O	-0.0532475	-1.9766112	2.4236182
O	0.7496709	-3.1478094	-0.3379559

C_3B

Mg	0.0000000	0.0000000	-0.2102142
Mg	0.2166288	1.9311531	-2.2837315
Mg	1.7346036	2.3658355	-0.0551387
Mg	-1.1485575	2.7061851	-0.0459345
Mg	-2.9161755	0.3192930	-0.0551387
Mg	1.4921797	0.6472411	2.1671258
Mg	-1.3066171	0.9686450	2.1671258
Mg	2.9179038	-0.3584126	-0.0459345
Mg	1.5641133	-1.1531826	-2.2837315
Mg	1.1815719	-2.6851286	-0.0551387
Mg	-1.7807421	-0.7779705	-2.2837315
Mg	-1.7693463	-2.3477725	-0.0459345
Mg	-0.1855626	-1.6158861	2.1671258
O	0.3872662	3.3860780	-1.1245374
O	2.9803664	1.2899091	0.9680708
O	0.0000000	0.0000000	3.2769400
O	1.3517415	-1.0034814	0.9921879
O	2.7387964	-2.0284213	-1.1245374
O	-2.6072772	1.9361185	0.9680708
O	0.1931696	1.6723832	0.9921879
O	-1.3682635	1.0096174	-1.6402843
O	1.5584861	0.6801422	-1.6402843
O	-3.1260626	-1.3576566	-1.1245374
O	-0.1902226	-1.6897597	-1.6402843
O	-1.5449111	-0.6689018	0.9921879
O	-0.3730892	-3.2260275	0.9680708

$(MgO)_{14}$:

C_1A

Mg	2.1252490	1.4952255	1.0759189
Mg	0.6904215	-2.0274471	1.0183500
Mg	-0.6346838	0.0042473	2.2652193
Mg	3.0831874	-0.9342839	1.7669108
Mg	-0.8413106	2.8709286	0.9724305
Mg	-3.3744172	0.8917407	0.9390153
Mg	-2.6990669	-2.1427375	0.9374996
Mg	-4.0098183	-0.8296562	-0.9236092
Mg	-1.7630641	1.4861606	-1.7778451
Mg	0.9567915	2.9796835	-0.8932729
Mg	3.7447937	0.4742863	-0.9319801
Mg	1.2685570	-0.1803102	-1.9359938
Mg	2.5517950	-2.4447986	-0.8976181
Mg	-1.0754222	-1.6550390	-1.7168551
O	1.0498092	3.0733662	1.0478657
O	-0.9379160	3.0034338	-0.9721493
O	-4.1235248	-0.8642264	1.0233688
O	-3.4421400	0.9848828	-1.0149163
O	-1.7996802	1.4775765	1.8516553
O	-2.7285155	-2.2457457	-1.0291046
O	3.8866912	0.5773223	0.9636665
O	1.2620539	-0.1392602	1.8953764
O	2.5949333	-2.5911417	1.0068802
O	-1.0602003	-1.8126049	1.7966295

O	2.0880686	1.4786775	-1.1231762
O	3.1438719	-0.9983010	-1.9500689
O	0.6576220	-2.0121354	-0.9843367
O	-0.6140841	0.0801551	-2.4098603

C_1B

Mg	-0.4697497	-1.8216799	0.9370104
Mg	-2.6775954	1.2086284	0.9494527
Mg	-0.4146585	1.2319325	2.3429942
Mg	-3.1503800	-1.3788478	1.3560282
Mg	2.2888848	-0.4676002	2.3026687
Mg	2.0690121	2.2547013	0.6871956
Mg	-0.9576686	2.8615078	-0.2567101
Mg	1.7361225	1.8945029	-1.9062366
Mg	3.9444738	-0.1916144	-0.3630532
Mg	2.7998078	-2.3605969	0.5934174
Mg	-1.0315457	0.0857242	-2.0856542
Mg	-1.9884491	-2.3970155	-1.2995651
Mg	1.4226603	-1.1619854	-1.9485200
Mg	-3.6506743	0.2271096	-1.3326225
O	-2.2223092	-2.7847438	0.5412783
O	-1.5588054	-0.2829901	1.8556100
O	-4.1389823	0.0180826	0.5010839
O	-1.5010744	2.5896026	1.5563292
O	1.2797644	-2.0157618	1.7015161
O	3.8939211	-0.9465630	1.3910253
O	0.8667336	3.0298742	-0.6205873
O	3.2005418	1.5031002	-0.6966013
O	3.0552687	-1.7239803	-1.2023661
O	1.4836866	1.2608743	2.2294217
O	-0.2361186	-1.5922555	-1.0909675
O	0.7802919	0.4876400	-2.7149136
O	-2.7059606	-1.0074240	-2.3831181
O	-2.1172006	1.4797802	-1.0441150

C_1C

Mg	-0.4451820	-2.3229725	0.8893990
Mg	1.3686770	-2.8729061	-1.0574259
Mg	0.2726252	-0.6506182	-2.1969320
Mg	2.4458587	2.3876938	-0.7177811
Mg	3.9080398	1.1204236	0.9994827
Mg	2.9229753	0.0323447	-1.8215993
Mg	1.9790700	-1.7961235	1.9898586
Mg	-3.1628318	1.0953522	-1.7663812
Mg	-2.2342780	-1.3745114	-1.0713036
Mg	1.2496997	0.9207844	1.7136048
Mg	-1.4548198	-0.0289528	2.0016915
Mg	-0.6202670	1.6599275	-0.9666748
Mg	-3.8764576	-0.4595238	0.8938745
Mg	-2.3603042	2.3150553	1.0105403
O	-0.4725938	-2.2412478	-1.1541637
O	2.0402328	-1.5537382	-2.2600336
O	1.3664405	-3.1596518	0.8167438
O	4.0356772	1.2610147	-0.9324106
O	1.2097196	1.1850306	-1.6305254
O	3.0121317	-0.2643265	1.8591312
O	2.4412834	2.3967939	1.1523935
O	-2.2575800	-1.5669053	0.9527334
O	-1.4614532	0.1989683	-2.0972628
O	-4.0079752	-0.4261129	-0.9997722
O	-0.5593113	1.5188592	1.0451256
O	-3.2033874	0.9307169	2.0068745
O	0.2643783	-0.8938253	2.2076561
O	-2.4003693	2.5884508	-0.8668472

$(MgO)_{15}$:

D_{3h}

Mg	-1.0093875	-1.7483104	1.9670713
Mg	0.9959108	-1.7249682	0.0000000
Mg	0.9114760	-1.5787228	3.8911028
Mg	-1.8229520	0.0000000	3.8911028
Mg	-1.9918217	0.0000000	0.0000000
Mg	-1.0093875	1.7483104	-1.9670713
Mg	-1.8229520	0.0000000	-3.8911028
Mg	0.9959108	1.7249682	0.0000000
Mg	0.9114760	1.5787228	-3.8911028
Mg	0.9114760	1.5787228	3.8911028
Mg	-1.0093875	1.7483104	1.9670713
Mg	2.0187750	0.0000000	1.9670713
Mg	2.0187750	0.0000000	-1.9670713
Mg	0.9114760	-1.5787228	-3.8911028
Mg	-1.0093875	-1.7483104	-1.9670713
O	-0.9852327	-1.7064730	3.9725003
O	-2.0771376	0.0000000	1.9546161
O	1.0385688	-1.7988539	1.9546161
O	-0.9852327	1.7064730	3.9725003
O	1.9704653	0.0000000	3.9725003
O	1.0385688	1.7988539	-1.9546161
O	1.0385688	1.7988539	1.9546161
O	-2.0771376	0.0000000	-1.9546161
O	-0.9852327	1.7064730	-3.9725003
O	2.0887751	0.0000000	0.0000000
O	-1.0443876	1.8089323	0.0000000
O	-1.0443876	-1.8089323	0.0000000
O	1.0385688	-1.7988539	-1.9546161
O	1.9704653	0.0000000	-3.9725003
O	-0.9852327	-1.7064730	-3.9725003

C_{3h}

Mg	2.5591209	0.9379210	1.5913048
Mg	2.5591209	0.9379210	-1.5913048
Mg	1.6124743	-0.9328631	-3.2063250
Mg	-0.4672971	-2.6852242	-1.5913048
Mg	2.2022077	-1.8767966	0.0000000
Mg	-1.6141203	-0.9300122	-3.2063250
Mg	0.0016460	1.8628753	-3.2063250
Mg	0.5242497	2.8455661	0.0000000
Mg	-0.4672971	-2.6852242	1.5913048
Mg	-1.6141203	-0.9300122	3.2063250
Mg	-2.7264574	-0.9687695	0.0000000
Mg	-2.0918238	1.7473032	-1.5913048
Mg	-2.0918238	1.7473032	1.5913048
Mg	1.6124743	-0.9328631	3.2063250
Mg	0.0016460	1.8628753	3.2063250
O	2.6720947	-0.9902648	1.6056088
O	2.6720947	-0.9902648	-1.6056088
O	0.0345028	-1.9482428	-3.3082972
O	0.5528177	-2.9135331	0.0000000
O	1.6699764	1.0040017	-3.3082972
O	-1.7044792	0.9442411	-3.3082972
O	2.2467848	1.9355207	0.0000000
O	0.0345028	-1.9482428	3.3082972
O	-2.1936418	-1.8189694	1.6056088
O	-2.1936418	-1.8189694	-1.6056088

O	-1.7044792	0.9442411	3.3082972
O	-0.4784528	2.8092343	-1.6056088
O	-2.7996025	0.9780124	0.0000000
O	1.6699764	1.0040017	3.3082972
O	-0.4784528	2.8092343	1.6056088

$(MgO)_{16}$:

C_2

Mg	-0.9954989	1.0199202	2.8212574
Mg	-2.8909106	-0.8728204	2.7296787
Mg	0.9819534	1.0734927	0.8049437
Mg	2.8909106	0.8728204	2.7296787
Mg	1.0201479	-1.9646576	-0.9639693
Mg	2.9338892	-0.8995286	-2.5188018
Mg	3.0350657	-1.0701941	0.8176802
Mg	0.9954989	-1.0199202	2.8212574
Mg	2.9222893	1.8080808	-0.9584182
Mg	0.9859477	1.0064854	-2.7043654
Mg	-3.0350657	1.0701941	0.8176802
Mg	-0.9819534	-1.0734927	0.8049437
Mg	-2.9222893	-1.8080808	-0.9584182
Mg	-2.9338892	0.8995286	-2.5188018
Mg	-1.0201479	1.9646576	-0.9639693
Mg	-0.9859477	-1.0064854	-2.7043654
O	3.1067779	1.0740783	0.8042315
O	2.9581338	-1.0247270	2.8067541
O	-0.9743318	-1.1092480	2.8801446
O	-2.9581338	1.0247270	2.8067541
O	0.9743318	1.1092480	2.8801446
O	-0.9979370	1.0168011	0.7859613
O	0.9810396	2.0618803	-0.9475856
O	2.9969626	0.9957225	-2.6648305
O	3.0211987	-1.9150236	-0.9258307
O	0.9979370	-1.0168011	0.7859613
O	-3.0211987	1.9150236	-0.9258307
O	-2.9969626	-0.9957225	-2.6648305
O	0.9833440	-1.0364908	-2.7668501
O	-3.1067779	-1.0740783	0.8042315
O	-0.9810396	-2.0618803	-0.9475856
O	-0.9833440	1.0364908	-2.7668501

C_{3v}

Mg	1.7747062	-3.0738813	0.9166782
Mg	2.4374765	1.5836858	-1.8192243
Mg	0.1527739	2.9027595	-1.8192243
Mg	1.7747062	3.0738813	0.9166782
Mg	0.9042919	1.5662796	2.8787951
Mg	-2.5902504	1.3190737	-1.8192243
Mg	3.0572607	0.0000000	0.9798807
Mg	2.4374765	-1.5836858	-1.8192243
Mg	-2.5902504	-1.3190737	-1.8192243
Mg	0.0000000	0.0000000	-3.3838769
Mg	-1.5286304	-2.6476655	0.9798807
Mg	0.1527739	-2.9027595	-1.8192243
Mg	-1.8085839	0.0000000	2.8787951
Mg	-1.5286304	2.6476655	0.9798807
Mg	-3.5494124	0.0000000	0.9166782
Mg	0.9042919	-1.5662796	2.8787951
O	0.9265883	1.6048980	-3.0106301
O	1.8461223	-3.1975777	-0.9369795
O	3.1135108	0.0000000	-0.9780815
O	-1.8531765	0.0000000	-3.0106301
O	0.1102176	3.0104803	1.8814018
O	2.5520436	-1.6006914	1.8814018
O	-1.5567554	2.6963794	-0.9780815
O	1.8461223	3.1975777	-0.9369795
O	2.5520436	1.6006914	1.8814018
O	0.9265883	-1.6048980	-3.0106301
O	-1.5567554	-2.6963794	-0.9780815
O	0.1102176	-3.0104803	1.8814018
O	-3.6922447	0.0000000	-0.9369795
O	-2.6622612	1.4097889	1.8814018
O	-2.6622612	-1.4097889	1.8814018
O	0.0000000	0.0000000	3.4618231