

**Optical resonance coupling in compositionally different nanocube-nanosphere heterodimers**

Mufasila Mumthaz Muhammed & Junais Habeeb Mokkath

[j.mokath@kcst.edu.kw](mailto:j.mokath@kcst.edu.kw)

Quantum Nanophotonics Simulations Lab, Department of Physics, Kuwait College of Science And  
Technology, Doha Area, 7th Ring Road, P.O. Box 27235, Kuwait

Atomic coordinates (d = 3Å)

Mg	1.000000e+01	1.004000e+01	1.000000e+01
Mg	1.420000e+01	1.004000e+01	1.000000e+01
Mg	1.840000e+01	1.004000e+01	1.000000e+01
Mg	2.260000e+01	1.004000e+01	1.000000e+01
Mg	1.000000e+01	1.424000e+01	1.000000e+01
Mg	1.420000e+01	1.424000e+01	1.000000e+01
Mg	1.840000e+01	1.424000e+01	1.000000e+01
Mg	2.260000e+01	1.424000e+01	1.000000e+01
Mg	1.000000e+01	1.844000e+01	1.000000e+01
Mg	1.420000e+01	1.844000e+01	1.000000e+01
Mg	1.840000e+01	1.844000e+01	1.000000e+01
Mg	2.260000e+01	1.844000e+01	1.000000e+01
Mg	1.000000e+01	2.264000e+01	1.000000e+01
Mg	1.420000e+01	2.264000e+01	1.000000e+01
Mg	1.840000e+01	2.264000e+01	1.000000e+01
Mg	2.260000e+01	2.264000e+01	1.000000e+01
Mg	1.000000e+01	1.004000e+01	1.420000e+01
Mg	1.420000e+01	1.004000e+01	1.420000e+01
Mg	1.840000e+01	1.004000e+01	1.420000e+01
Mg	2.260000e+01	1.004000e+01	1.420000e+01
Mg	1.000000e+01	1.424000e+01	1.420000e+01
Mg	1.210000e+01	1.214000e+01	1.210000e+01
Mg	1.420000e+01	1.424000e+01	1.420000e+01
Mg	1.630000e+01	1.214000e+01	1.210000e+01
Mg	1.840000e+01	1.424000e+01	1.420000e+01
Mg	2.050000e+01	1.214000e+01	1.210000e+01
Mg	2.260000e+01	1.424000e+01	1.420000e+01
Mg	1.000000e+01	1.844000e+01	1.420000e+01
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Mg	2.260000e+01	1.844000e+01	1.420000e+01
Mg	1.000000e+01	2.264000e+01	1.420000e+01
Mg	1.210000e+01	2.054000e+01	1.210000e+01
Mg	1.420000e+01	2.264000e+01	1.420000e+01
Mg	1.630000e+01	2.054000e+01	1.210000e+01
Mg	1.840000e+01	2.264000e+01	1.420000e+01
Mg	2.050000e+01	2.054000e+01	1.210000e+01
Mg	2.260000e+01	2.264000e+01	1.420000e+01
Mg	1.000000e+01	1.004000e+01	1.840000e+01
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Mg	2.260000e+01	2.264000e+01	1.840000e+01
Mg	1.000000e+01	1.004000e+01	2.260000e+01
Mg	1.420000e+01	1.004000e+01	2.260000e+01
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Mg	2.050000e+01	2.054000e+01	2.050000e+01
Mg	2.260000e+01	2.264000e+01	2.260000e+01
Mg	1.424000e+01	1.421000e+01	2.560000e+01
Mg	1.844000e+01	1.421000e+01	2.560000e+01
Mg	1.424000e+01	1.841000e+01	2.560000e+01
Mg	1.844000e+01	1.841000e+01	2.560000e+01
Mg	1.424000e+01	1.001000e+01	2.980000e+01

Mg 1.844000e+01 1.001000e+01 2.980000e+01  
Mg 1.004000e+01 1.421000e+01 2.980000e+01  
Mg 1.424000e+01 1.421000e+01 2.980000e+01  
Mg 1.634000e+01 1.211000e+01 2.770000e+01  
Mg 1.844000e+01 1.421000e+01 2.980000e+01  
Mg 2.264000e+01 1.421000e+01 2.980000e+01  
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Mg	2.054000e+01	2.051000e+01	3.190000e+01
Mg	1.424000e+01	1.421000e+01	3.820000e+01
Mg	1.634000e+01	1.211000e+01	3.610000e+01
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Mg	1.634000e+01	1.631000e+01	3.610000e+01
Mg	1.844000e+01	1.841000e+01	3.820000e+01
Mg	2.054000e+01	1.631000e+01	3.610000e+01
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Atomic coordinates (d = 4A)

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Mg	1.840000e+01	2.264000e+01	1.000000e+01
Mg	2.260000e+01	2.264000e+01	1.000000e+01
Mg	1.000000e+01	1.004000e+01	1.420000e+01

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Mg	1.840000e+01	2.264000e+01	1.840000e+01
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Mg 1.634000e+01 1.211000e+01 3.710000e+01  
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Mg	2.260000e+01	1.004000e+01	1.420000e+01
Mg	1.000000e+01	1.424000e+01	1.420000e+01
Mg	1.210000e+01	1.214000e+01	1.210000e+01
Mg	1.420000e+01	1.424000e+01	1.420000e+01
Mg	1.630000e+01	1.214000e+01	1.210000e+01
Mg	1.840000e+01	1.424000e+01	1.420000e+01
Mg	2.050000e+01	1.214000e+01	1.210000e+01
Mg	2.260000e+01	1.424000e+01	1.420000e+01
Mg	1.000000e+01	1.844000e+01	1.420000e+01
Mg	1.210000e+01	1.634000e+01	1.210000e+01
Mg	1.420000e+01	1.844000e+01	1.420000e+01
Mg	1.630000e+01	1.634000e+01	1.210000e+01
Mg	1.840000e+01	1.844000e+01	1.420000e+01
Mg	2.050000e+01	1.634000e+01	1.210000e+01
Mg	2.260000e+01	1.844000e+01	1.420000e+01
Mg	1.000000e+01	2.264000e+01	1.420000e+01
Mg	1.210000e+01	2.054000e+01	1.210000e+01

Mg	1.420000e+01	2.264000e+01	1.420000e+01
Mg	1.630000e+01	2.054000e+01	1.210000e+01
Mg	1.840000e+01	2.264000e+01	1.420000e+01
Mg	2.050000e+01	2.054000e+01	1.210000e+01
Mg	2.260000e+01	2.264000e+01	1.420000e+01
Mg	1.000000e+01	1.004000e+01	1.840000e+01
Mg	1.420000e+01	1.004000e+01	1.840000e+01
Mg	1.840000e+01	1.004000e+01	1.840000e+01
Mg	2.260000e+01	1.004000e+01	1.840000e+01
Mg	1.000000e+01	1.424000e+01	1.840000e+01
Mg	1.210000e+01	1.214000e+01	1.630000e+01
Mg	1.420000e+01	1.424000e+01	1.840000e+01
Mg	1.630000e+01	1.214000e+01	1.630000e+01
Mg	1.840000e+01	1.424000e+01	1.840000e+01
Mg	2.050000e+01	1.214000e+01	1.630000e+01
Mg	2.260000e+01	1.424000e+01	1.840000e+01
Mg	1.000000e+01	1.844000e+01	1.840000e+01
Mg	1.210000e+01	1.634000e+01	1.630000e+01
Mg	1.420000e+01	1.844000e+01	1.840000e+01
Mg	1.630000e+01	1.634000e+01	1.630000e+01
Mg	1.840000e+01	1.844000e+01	1.840000e+01
Mg	2.050000e+01	1.634000e+01	1.630000e+01
Mg	2.260000e+01	1.844000e+01	1.840000e+01
Mg	1.000000e+01	2.264000e+01	1.840000e+01
Mg	1.210000e+01	2.054000e+01	1.630000e+01
Mg	1.420000e+01	2.264000e+01	1.840000e+01
Mg	1.630000e+01	2.054000e+01	1.630000e+01
Mg	1.840000e+01	2.264000e+01	1.840000e+01
Mg	2.050000e+01	2.054000e+01	1.630000e+01
Mg	2.260000e+01	2.264000e+01	1.840000e+01
Mg	1.000000e+01	1.004000e+01	2.260000e+01
Mg	1.420000e+01	1.004000e+01	2.260000e+01
Mg	1.840000e+01	1.004000e+01	2.260000e+01

Mg 2.260000e+01 1.004000e+01 2.260000e+01  
Mg 1.000000e+01 1.424000e+01 2.260000e+01  
Mg 1.210000e+01 1.214000e+01 2.050000e+01  
Mg 1.420000e+01 1.424000e+01 2.260000e+01  
Mg 1.630000e+01 1.214000e+01 2.050000e+01  
Mg 1.840000e+01 1.424000e+01 2.260000e+01  
Mg 2.050000e+01 1.214000e+01 2.050000e+01  
Mg 2.260000e+01 1.424000e+01 2.260000e+01  
Mg 1.000000e+01 1.844000e+01 2.260000e+01  
Mg 1.210000e+01 1.634000e+01 2.050000e+01  
Mg 1.420000e+01 1.844000e+01 2.260000e+01  
Mg 1.630000e+01 1.634000e+01 2.050000e+01  
Mg 1.840000e+01 1.844000e+01 2.260000e+01  
Mg 2.050000e+01 1.634000e+01 2.050000e+01  
Mg 2.260000e+01 1.844000e+01 2.260000e+01  
Mg 1.000000e+01 2.264000e+01 2.260000e+01  
Mg 1.210000e+01 2.054000e+01 2.050000e+01  
Mg 1.420000e+01 2.264000e+01 2.260000e+01  
Mg 1.630000e+01 2.054000e+01 2.050000e+01  
Mg 1.840000e+01 2.264000e+01 2.260000e+01  
Mg 2.050000e+01 2.054000e+01 2.050000e+01  
Mg 2.260000e+01 2.264000e+01 2.260000e+01  
Mg 1.424000e+01 1.421000e+01 2.760000e+01  
Mg 1.844000e+01 1.421000e+01 2.760000e+01  
Mg 1.424000e+01 1.841000e+01 2.760000e+01  
Mg 1.844000e+01 1.841000e+01 2.760000e+01  
Mg 1.424000e+01 1.001000e+01 3.180000e+01  
Mg 1.844000e+01 1.001000e+01 3.180000e+01  
Mg 1.004000e+01 1.421000e+01 3.180000e+01  
Mg 1.424000e+01 1.421000e+01 3.180000e+01  
Mg 1.634000e+01 1.211000e+01 2.970000e+01  
Mg 1.844000e+01 1.421000e+01 3.180000e+01  
Mg 2.264000e+01 1.421000e+01 3.180000e+01

Mg	1.004000e+01	1.841000e+01	3.180000e+01
Mg	1.214000e+01	1.631000e+01	2.970000e+01
Mg	1.424000e+01	1.841000e+01	3.180000e+01
Mg	1.634000e+01	1.631000e+01	2.970000e+01
Mg	1.844000e+01	1.841000e+01	3.180000e+01
Mg	2.054000e+01	1.631000e+01	2.970000e+01
Mg	2.264000e+01	1.841000e+01	3.180000e+01
Mg	1.424000e+01	2.261000e+01	3.180000e+01
Mg	1.634000e+01	2.051000e+01	2.970000e+01
Mg	1.844000e+01	2.261000e+01	3.180000e+01
Mg	1.424000e+01	1.001000e+01	3.600000e+01
Mg	1.844000e+01	1.001000e+01	3.600000e+01
Mg	1.004000e+01	1.421000e+01	3.600000e+01
Mg	1.214000e+01	1.211000e+01	3.390000e+01
Mg	1.424000e+01	1.421000e+01	3.600000e+01
Mg	1.634000e+01	1.211000e+01	3.390000e+01
Mg	1.844000e+01	1.421000e+01	3.600000e+01
Mg	2.054000e+01	1.211000e+01	3.390000e+01
Mg	2.264000e+01	1.421000e+01	3.600000e+01
Mg	1.004000e+01	1.841000e+01	3.600000e+01
Mg	1.214000e+01	1.631000e+01	3.390000e+01
Mg	1.424000e+01	1.841000e+01	3.600000e+01
Mg	1.634000e+01	1.631000e+01	3.390000e+01
Mg	1.844000e+01	1.841000e+01	3.600000e+01
Mg	2.054000e+01	1.631000e+01	3.390000e+01
Mg	2.264000e+01	1.841000e+01	3.600000e+01
Mg	1.214000e+01	2.051000e+01	3.390000e+01
Mg	1.424000e+01	2.261000e+01	3.600000e+01
Mg	1.634000e+01	2.051000e+01	3.390000e+01
Mg	1.844000e+01	2.261000e+01	3.600000e+01
Mg	2.054000e+01	2.051000e+01	3.390000e+01
Mg	1.424000e+01	1.421000e+01	4.020000e+01
Mg	1.634000e+01	1.211000e+01	3.810000e+01

Mg	1.844000e+01	1.421000e+01	4.020000e+01
Mg	1.214000e+01	1.631000e+01	3.810000e+01
Mg	1.424000e+01	1.841000e+01	4.020000e+01
Mg	1.634000e+01	1.631000e+01	3.810000e+01
Mg	1.844000e+01	1.841000e+01	4.020000e+01
Mg	2.054000e+01	1.631000e+01	3.810000e+01
Mg	1.634000e+01	2.051000e+01	3.810000e+01

Atomic coordinates (d = 6Å)

Mg	1.000000e+01	1.004000e+01	1.000000e+01
Mg	1.420000e+01	1.004000e+01	1.000000e+01
Mg	1.840000e+01	1.004000e+01	1.000000e+01
Mg	2.260000e+01	1.004000e+01	1.000000e+01
Mg	1.000000e+01	1.424000e+01	1.000000e+01
Mg	1.420000e+01	1.424000e+01	1.000000e+01
Mg	1.840000e+01	1.424000e+01	1.000000e+01
Mg	2.260000e+01	1.424000e+01	1.000000e+01
Mg	1.000000e+01	1.844000e+01	1.000000e+01
Mg	1.420000e+01	1.844000e+01	1.000000e+01
Mg	1.840000e+01	1.844000e+01	1.000000e+01
Mg	2.260000e+01	1.844000e+01	1.000000e+01
Mg	1.000000e+01	2.264000e+01	1.000000e+01
Mg	1.420000e+01	2.264000e+01	1.000000e+01
Mg	1.840000e+01	2.264000e+01	1.000000e+01
Mg	2.260000e+01	2.264000e+01	1.000000e+01
Mg	1.000000e+01	1.004000e+01	1.420000e+01
Mg	1.420000e+01	1.004000e+01	1.420000e+01
Mg	1.840000e+01	1.004000e+01	1.420000e+01
Mg	2.260000e+01	1.004000e+01	1.420000e+01
Mg	1.000000e+01	1.424000e+01	1.420000e+01
Mg	1.210000e+01	1.214000e+01	1.210000e+01
Mg	1.420000e+01	1.424000e+01	1.420000e+01

Mg	1.630000e+01	1.214000e+01	1.210000e+01
Mg	1.840000e+01	1.424000e+01	1.420000e+01
Mg	2.050000e+01	1.214000e+01	1.210000e+01
Mg	2.260000e+01	1.424000e+01	1.420000e+01
Mg	1.000000e+01	1.844000e+01	1.420000e+01
Mg	1.210000e+01	1.634000e+01	1.210000e+01
Mg	1.420000e+01	1.844000e+01	1.420000e+01
Mg	1.630000e+01	1.634000e+01	1.210000e+01
Mg	1.840000e+01	1.844000e+01	1.420000e+01
Mg	2.050000e+01	1.634000e+01	1.210000e+01
Mg	2.260000e+01	1.844000e+01	1.420000e+01
Mg	1.000000e+01	2.264000e+01	1.420000e+01
Mg	1.210000e+01	2.054000e+01	1.210000e+01
Mg	1.420000e+01	2.264000e+01	1.420000e+01
Mg	1.630000e+01	2.054000e+01	1.210000e+01
Mg	1.840000e+01	2.264000e+01	1.420000e+01
Mg	2.050000e+01	2.054000e+01	1.210000e+01
Mg	2.260000e+01	2.264000e+01	1.420000e+01
Mg	1.000000e+01	1.004000e+01	1.840000e+01
Mg	1.420000e+01	1.004000e+01	1.840000e+01
Mg	1.840000e+01	1.004000e+01	1.840000e+01
Mg	2.260000e+01	1.004000e+01	1.840000e+01
Mg	1.000000e+01	1.424000e+01	1.840000e+01
Mg	1.210000e+01	1.214000e+01	1.630000e+01
Mg	1.420000e+01	1.424000e+01	1.840000e+01
Mg	1.630000e+01	1.214000e+01	1.630000e+01
Mg	1.840000e+01	1.424000e+01	1.840000e+01
Mg	2.050000e+01	1.214000e+01	1.630000e+01
Mg	2.260000e+01	1.424000e+01	1.840000e+01
Mg	1.000000e+01	1.844000e+01	1.840000e+01
Mg	1.210000e+01	1.634000e+01	1.630000e+01
Mg	1.420000e+01	1.844000e+01	1.840000e+01
Mg	1.630000e+01	1.634000e+01	1.630000e+01

Mg	1.840000e+01	1.844000e+01	1.840000e+01
Mg	2.050000e+01	1.634000e+01	1.630000e+01
Mg	2.260000e+01	1.844000e+01	1.840000e+01
Mg	1.000000e+01	2.264000e+01	1.840000e+01
Mg	1.210000e+01	2.054000e+01	1.630000e+01
Mg	1.420000e+01	2.264000e+01	1.840000e+01
Mg	1.630000e+01	2.054000e+01	1.630000e+01
Mg	1.840000e+01	2.264000e+01	1.840000e+01
Mg	2.050000e+01	2.054000e+01	1.630000e+01
Mg	2.260000e+01	2.264000e+01	1.840000e+01
Mg	1.000000e+01	1.004000e+01	2.260000e+01
Mg	1.420000e+01	1.004000e+01	2.260000e+01
Mg	1.840000e+01	1.004000e+01	2.260000e+01
Mg	2.260000e+01	1.004000e+01	2.260000e+01
Mg	1.000000e+01	1.424000e+01	2.260000e+01
Mg	1.210000e+01	1.214000e+01	2.050000e+01
Mg	1.420000e+01	1.424000e+01	2.260000e+01
Mg	1.630000e+01	1.214000e+01	2.050000e+01
Mg	1.840000e+01	1.424000e+01	2.260000e+01
Mg	2.050000e+01	1.214000e+01	2.050000e+01
Mg	2.260000e+01	1.424000e+01	2.260000e+01
Mg	1.000000e+01	1.844000e+01	2.260000e+01
Mg	1.210000e+01	1.634000e+01	2.050000e+01
Mg	1.420000e+01	1.844000e+01	2.260000e+01
Mg	1.630000e+01	1.634000e+01	2.050000e+01
Mg	1.840000e+01	1.844000e+01	2.260000e+01
Mg	2.050000e+01	1.634000e+01	2.050000e+01
Mg	2.260000e+01	1.844000e+01	2.260000e+01
Mg	1.000000e+01	2.264000e+01	2.260000e+01
Mg	1.210000e+01	2.054000e+01	2.050000e+01
Mg	1.420000e+01	2.264000e+01	2.260000e+01
Mg	1.630000e+01	2.054000e+01	2.050000e+01
Mg	1.840000e+01	2.264000e+01	2.260000e+01

Mg 2.050000e+01 2.054000e+01 2.050000e+01  
Mg 2.260000e+01 2.264000e+01 2.260000e+01  
Mg 1.424000e+01 1.421000e+01 2.860000e+01  
Mg 1.844000e+01 1.421000e+01 2.860000e+01  
Mg 1.424000e+01 1.841000e+01 2.860000e+01  
Mg 1.844000e+01 1.841000e+01 2.860000e+01  
Mg 1.424000e+01 1.001000e+01 3.280000e+01  
Mg 1.844000e+01 1.001000e+01 3.280000e+01  
Mg 1.004000e+01 1.421000e+01 3.280000e+01  
Mg 1.424000e+01 1.421000e+01 3.280000e+01  
Mg 1.634000e+01 1.211000e+01 3.070000e+01  
Mg 1.844000e+01 1.421000e+01 3.280000e+01  
Mg 2.264000e+01 1.421000e+01 3.280000e+01  
Mg 1.004000e+01 1.841000e+01 3.280000e+01  
Mg 1.214000e+01 1.631000e+01 3.070000e+01  
Mg 1.424000e+01 1.841000e+01 3.280000e+01  
Mg 1.634000e+01 1.631000e+01 3.070000e+01  
Mg 1.844000e+01 1.841000e+01 3.280000e+01  
Mg 2.054000e+01 1.631000e+01 3.070000e+01  
Mg 2.264000e+01 1.841000e+01 3.280000e+01  
Mg 1.424000e+01 2.261000e+01 3.280000e+01  
Mg 1.634000e+01 2.051000e+01 3.070000e+01  
Mg 1.844000e+01 2.261000e+01 3.280000e+01  
Mg 1.424000e+01 1.001000e+01 3.700000e+01  
Mg 1.844000e+01 1.001000e+01 3.700000e+01  
Mg 1.004000e+01 1.421000e+01 3.700000e+01  
Mg 1.214000e+01 1.211000e+01 3.490000e+01  
Mg 1.424000e+01 1.421000e+01 3.700000e+01  
Mg 1.634000e+01 1.211000e+01 3.490000e+01  
Mg 1.844000e+01 1.421000e+01 3.700000e+01  
Mg 2.054000e+01 1.211000e+01 3.490000e+01  
Mg 2.264000e+01 1.421000e+01 3.700000e+01  
Mg 1.004000e+01 1.841000e+01 3.700000e+01

Mg 1.214000e+01 1.631000e+01 3.490000e+01  
Mg 1.424000e+01 1.841000e+01 3.700000e+01  
Mg 1.634000e+01 1.631000e+01 3.490000e+01  
Mg 1.844000e+01 1.841000e+01 3.700000e+01  
Mg 2.054000e+01 1.631000e+01 3.490000e+01  
Mg 2.264000e+01 1.841000e+01 3.700000e+01  
Mg 1.214000e+01 2.051000e+01 3.490000e+01  
Mg 1.424000e+01 2.261000e+01 3.700000e+01  
Mg 1.634000e+01 2.051000e+01 3.490000e+01  
Mg 1.844000e+01 2.261000e+01 3.700000e+01  
Mg 2.054000e+01 2.051000e+01 3.490000e+01  
Mg 1.424000e+01 1.421000e+01 4.120000e+01  
Mg 1.634000e+01 1.211000e+01 3.910000e+01  
Mg 1.844000e+01 1.421000e+01 4.120000e+01  
Mg 1.214000e+01 1.631000e+01 3.910000e+01  
Mg 1.424000e+01 1.841000e+01 4.120000e+01  
Mg 1.634000e+01 1.631000e+01 3.910000e+01  
Mg 1.844000e+01 1.841000e+01 4.120000e+01  
Mg 2.054000e+01 1.631000e+01 3.910000e+01  
Mg 1.634000e+01 2.051000e+01 3.910000e+01

Atomic coordinates (d = 7Å)

Mg 1.000000e+01 1.004000e+01 1.000000e+01  
Mg 1.420000e+01 1.004000e+01 1.000000e+01  
Mg 1.840000e+01 1.004000e+01 1.000000e+01  
Mg 2.260000e+01 1.004000e+01 1.000000e+01  
Mg 1.000000e+01 1.424000e+01 1.000000e+01  
Mg 1.420000e+01 1.424000e+01 1.000000e+01  
Mg 1.840000e+01 1.424000e+01 1.000000e+01  
Mg 2.260000e+01 1.424000e+01 1.000000e+01  
Mg 1.000000e+01 1.844000e+01 1.000000e+01  
Mg 1.420000e+01 1.844000e+01 1.000000e+01

Mg	1.840000e+01	1.844000e+01	1.000000e+01
Mg	2.260000e+01	1.844000e+01	1.000000e+01
Mg	1.000000e+01	2.264000e+01	1.000000e+01
Mg	1.420000e+01	2.264000e+01	1.000000e+01
Mg	1.840000e+01	2.264000e+01	1.000000e+01
Mg	2.260000e+01	2.264000e+01	1.000000e+01
Mg	1.000000e+01	1.004000e+01	1.420000e+01
Mg	1.420000e+01	1.004000e+01	1.420000e+01
Mg	1.840000e+01	1.004000e+01	1.420000e+01
Mg	2.260000e+01	1.004000e+01	1.420000e+01
Mg	1.000000e+01	1.424000e+01	1.420000e+01
Mg	1.210000e+01	1.214000e+01	1.210000e+01
Mg	1.420000e+01	1.424000e+01	1.420000e+01
Mg	1.630000e+01	1.214000e+01	1.210000e+01
Mg	1.840000e+01	1.424000e+01	1.420000e+01
Mg	2.050000e+01	1.214000e+01	1.210000e+01
Mg	2.260000e+01	1.424000e+01	1.420000e+01
Mg	1.000000e+01	1.844000e+01	1.420000e+01
Mg	1.210000e+01	1.634000e+01	1.210000e+01
Mg	1.420000e+01	1.844000e+01	1.420000e+01
Mg	1.630000e+01	1.634000e+01	1.210000e+01
Mg	1.840000e+01	1.844000e+01	1.420000e+01
Mg	2.050000e+01	1.634000e+01	1.210000e+01
Mg	2.260000e+01	1.844000e+01	1.420000e+01
Mg	1.000000e+01	2.264000e+01	1.420000e+01
Mg	1.210000e+01	2.054000e+01	1.210000e+01
Mg	1.420000e+01	2.264000e+01	1.420000e+01
Mg	1.630000e+01	2.054000e+01	1.210000e+01
Mg	1.840000e+01	2.264000e+01	1.420000e+01
Mg	2.050000e+01	2.054000e+01	1.210000e+01
Mg	2.260000e+01	2.264000e+01	1.420000e+01
Mg	1.000000e+01	1.004000e+01	1.840000e+01
Mg	1.420000e+01	1.004000e+01	1.840000e+01

Mg	1.840000e+01	1.004000e+01	1.840000e+01
Mg	2.260000e+01	1.004000e+01	1.840000e+01
Mg	1.000000e+01	1.424000e+01	1.840000e+01
Mg	1.210000e+01	1.214000e+01	1.630000e+01
Mg	1.420000e+01	1.424000e+01	1.840000e+01
Mg	1.630000e+01	1.214000e+01	1.630000e+01
Mg	1.840000e+01	1.424000e+01	1.840000e+01
Mg	2.050000e+01	1.214000e+01	1.630000e+01
Mg	2.260000e+01	1.424000e+01	1.840000e+01
Mg	1.000000e+01	1.844000e+01	1.840000e+01
Mg	1.210000e+01	1.634000e+01	1.630000e+01
Mg	1.420000e+01	1.844000e+01	1.840000e+01
Mg	1.630000e+01	1.634000e+01	1.630000e+01
Mg	1.840000e+01	1.844000e+01	1.840000e+01
Mg	2.050000e+01	1.634000e+01	1.630000e+01
Mg	2.260000e+01	1.844000e+01	1.840000e+01
Mg	1.000000e+01	2.264000e+01	1.840000e+01
Mg	1.210000e+01	2.054000e+01	1.630000e+01
Mg	1.420000e+01	2.264000e+01	1.840000e+01
Mg	1.630000e+01	2.054000e+01	1.630000e+01
Mg	1.840000e+01	2.264000e+01	1.840000e+01
Mg	2.050000e+01	2.054000e+01	1.630000e+01
Mg	2.260000e+01	2.264000e+01	1.840000e+01
Mg	1.000000e+01	1.004000e+01	2.260000e+01
Mg	1.420000e+01	1.004000e+01	2.260000e+01
Mg	1.840000e+01	1.004000e+01	2.260000e+01
Mg	2.260000e+01	1.004000e+01	2.260000e+01
Mg	1.000000e+01	1.424000e+01	2.260000e+01
Mg	1.210000e+01	1.214000e+01	2.050000e+01
Mg	1.420000e+01	1.424000e+01	2.260000e+01
Mg	1.630000e+01	1.214000e+01	2.050000e+01
Mg	1.840000e+01	1.424000e+01	2.260000e+01
Mg	2.050000e+01	1.214000e+01	2.050000e+01

Mg 2.260000e+01 1.424000e+01 2.260000e+01  
Mg 1.000000e+01 1.844000e+01 2.260000e+01  
Mg 1.210000e+01 1.634000e+01 2.050000e+01  
Mg 1.420000e+01 1.844000e+01 2.260000e+01  
Mg 1.630000e+01 1.634000e+01 2.050000e+01  
Mg 1.840000e+01 1.844000e+01 2.260000e+01  
Mg 2.050000e+01 1.634000e+01 2.050000e+01  
Mg 2.260000e+01 1.844000e+01 2.260000e+01  
Mg 1.000000e+01 2.264000e+01 2.260000e+01  
Mg 1.210000e+01 2.054000e+01 2.050000e+01  
Mg 1.420000e+01 2.264000e+01 2.260000e+01  
Mg 1.630000e+01 2.054000e+01 2.050000e+01  
Mg 1.840000e+01 2.264000e+01 2.260000e+01  
Mg 2.050000e+01 2.054000e+01 2.050000e+01  
Mg 2.260000e+01 2.264000e+01 2.260000e+01  
Mg 1.424000e+01 1.421000e+01 2.960000e+01  
Mg 1.844000e+01 1.421000e+01 2.960000e+01  
Mg 1.424000e+01 1.841000e+01 2.960000e+01  
Mg 1.844000e+01 1.841000e+01 2.960000e+01  
Mg 1.424000e+01 1.001000e+01 3.380000e+01  
Mg 1.844000e+01 1.001000e+01 3.380000e+01  
Mg 1.004000e+01 1.421000e+01 3.380000e+01  
Mg 1.424000e+01 1.421000e+01 3.380000e+01  
Mg 1.634000e+01 1.211000e+01 3.170000e+01  
Mg 1.844000e+01 1.421000e+01 3.380000e+01  
Mg 2.264000e+01 1.421000e+01 3.380000e+01  
Mg 1.004000e+01 1.841000e+01 3.380000e+01  
Mg 1.214000e+01 1.631000e+01 3.170000e+01  
Mg 1.424000e+01 1.841000e+01 3.380000e+01  
Mg 1.634000e+01 1.631000e+01 3.170000e+01  
Mg 1.844000e+01 1.841000e+01 3.380000e+01  
Mg 2.054000e+01 1.631000e+01 3.170000e+01  
Mg 2.264000e+01 1.841000e+01 3.380000e+01

Mg 1.424000e+01 2.261000e+01 3.380000e+01  
Mg 1.634000e+01 2.051000e+01 3.170000e+01  
Mg 1.844000e+01 2.261000e+01 3.380000e+01  
Mg 1.424000e+01 1.001000e+01 3.800000e+01  
Mg 1.844000e+01 1.001000e+01 3.800000e+01  
Mg 1.004000e+01 1.421000e+01 3.800000e+01  
Mg 1.214000e+01 1.211000e+01 3.590000e+01  
Mg 1.424000e+01 1.421000e+01 3.800000e+01  
Mg 1.634000e+01 1.211000e+01 3.590000e+01  
Mg 1.844000e+01 1.421000e+01 3.800000e+01  
Mg 2.054000e+01 1.211000e+01 3.590000e+01  
Mg 2.264000e+01 1.421000e+01 3.800000e+01  
Mg 1.004000e+01 1.841000e+01 3.800000e+01  
Mg 1.214000e+01 1.631000e+01 3.590000e+01  
Mg 1.424000e+01 1.841000e+01 3.800000e+01  
Mg 1.634000e+01 1.631000e+01 3.590000e+01  
Mg 1.844000e+01 1.841000e+01 3.800000e+01  
Mg 2.054000e+01 1.631000e+01 3.590000e+01  
Mg 2.264000e+01 1.841000e+01 3.800000e+01  
Mg 1.214000e+01 2.051000e+01 3.590000e+01  
Mg 1.424000e+01 2.261000e+01 3.800000e+01  
Mg 1.634000e+01 2.051000e+01 3.590000e+01  
Mg 1.844000e+01 2.261000e+01 3.800000e+01  
Mg 2.054000e+01 2.051000e+01 3.590000e+01  
Mg 1.424000e+01 1.421000e+01 4.220000e+01  
Mg 1.634000e+01 1.211000e+01 4.010000e+01  
Mg 1.844000e+01 1.421000e+01 4.220000e+01  
Mg 1.214000e+01 1.631000e+01 4.010000e+01  
Mg 1.424000e+01 1.841000e+01 4.220000e+01  
Mg 1.634000e+01 1.631000e+01 4.010000e+01  
Mg 1.844000e+01 1.841000e+01 4.220000e+01  
Mg 2.054000e+01 1.631000e+01 4.010000e+01  
Mg 1.634000e+01 2.051000e+01 4.010000e+01

Atomic coordinates (d = 8Å)

Mg	1.000000e+01	1.004000e+01	1.000000e+01
Mg	1.420000e+01	1.004000e+01	1.000000e+01
Mg	1.840000e+01	1.004000e+01	1.000000e+01
Mg	2.260000e+01	1.004000e+01	1.000000e+01
Mg	1.000000e+01	1.424000e+01	1.000000e+01
Mg	1.420000e+01	1.424000e+01	1.000000e+01
Mg	1.840000e+01	1.424000e+01	1.000000e+01
Mg	2.260000e+01	1.424000e+01	1.000000e+01
Mg	1.000000e+01	1.844000e+01	1.000000e+01
Mg	1.420000e+01	1.844000e+01	1.000000e+01
Mg	1.840000e+01	1.844000e+01	1.000000e+01
Mg	2.260000e+01	1.844000e+01	1.000000e+01
Mg	1.000000e+01	2.264000e+01	1.000000e+01
Mg	1.420000e+01	2.264000e+01	1.000000e+01
Mg	1.840000e+01	2.264000e+01	1.000000e+01
Mg	2.260000e+01	2.264000e+01	1.000000e+01
Mg	1.000000e+01	1.004000e+01	1.420000e+01
Mg	1.420000e+01	1.004000e+01	1.420000e+01
Mg	1.840000e+01	1.004000e+01	1.420000e+01
Mg	2.260000e+01	1.004000e+01	1.420000e+01
Mg	1.000000e+01	1.424000e+01	1.420000e+01
Mg	1.210000e+01	1.214000e+01	1.210000e+01
Mg	1.420000e+01	1.424000e+01	1.420000e+01
Mg	1.630000e+01	1.214000e+01	1.210000e+01
Mg	1.840000e+01	1.424000e+01	1.420000e+01
Mg	2.050000e+01	1.214000e+01	1.210000e+01
Mg	2.260000e+01	1.424000e+01	1.420000e+01
Mg	1.000000e+01	1.844000e+01	1.420000e+01
Mg	1.210000e+01	1.634000e+01	1.210000e+01
Mg	1.420000e+01	1.844000e+01	1.420000e+01

Mg	1.630000e+01	1.634000e+01	1.210000e+01
Mg	1.840000e+01	1.844000e+01	1.420000e+01
Mg	2.050000e+01	1.634000e+01	1.210000e+01
Mg	2.260000e+01	1.844000e+01	1.420000e+01
Mg	1.000000e+01	2.264000e+01	1.420000e+01
Mg	1.210000e+01	2.054000e+01	1.210000e+01
Mg	1.420000e+01	2.264000e+01	1.420000e+01
Mg	1.630000e+01	2.054000e+01	1.210000e+01
Mg	1.840000e+01	2.264000e+01	1.420000e+01
Mg	2.050000e+01	2.054000e+01	1.210000e+01
Mg	2.260000e+01	2.264000e+01	1.420000e+01
Mg	1.000000e+01	1.004000e+01	1.840000e+01
Mg	1.420000e+01	1.004000e+01	1.840000e+01
Mg	1.840000e+01	1.004000e+01	1.840000e+01
Mg	2.260000e+01	1.004000e+01	1.840000e+01
Mg	1.000000e+01	1.424000e+01	1.840000e+01
Mg	1.210000e+01	1.214000e+01	1.630000e+01
Mg	1.420000e+01	1.424000e+01	1.840000e+01
Mg	1.630000e+01	1.214000e+01	1.630000e+01
Mg	1.840000e+01	1.424000e+01	1.840000e+01
Mg	2.050000e+01	1.214000e+01	1.630000e+01
Mg	2.260000e+01	1.424000e+01	1.840000e+01
Mg	1.000000e+01	1.844000e+01	1.840000e+01
Mg	1.210000e+01	1.634000e+01	1.630000e+01
Mg	1.420000e+01	1.844000e+01	1.840000e+01
Mg	1.630000e+01	1.634000e+01	1.630000e+01
Mg	1.840000e+01	1.844000e+01	1.840000e+01
Mg	2.050000e+01	1.634000e+01	1.630000e+01
Mg	2.260000e+01	1.844000e+01	1.840000e+01
Mg	1.000000e+01	2.264000e+01	1.840000e+01
Mg	1.210000e+01	2.054000e+01	1.630000e+01
Mg	1.420000e+01	2.264000e+01	1.840000e+01
Mg	1.630000e+01	2.054000e+01	1.630000e+01

Mg 1.840000e+01 2.264000e+01 1.840000e+01  
Mg 2.050000e+01 2.054000e+01 1.630000e+01  
Mg 2.260000e+01 2.264000e+01 1.840000e+01  
Mg 1.000000e+01 1.004000e+01 2.260000e+01  
Mg 1.420000e+01 1.004000e+01 2.260000e+01  
Mg 1.840000e+01 1.004000e+01 2.260000e+01  
Mg 2.260000e+01 1.004000e+01 2.260000e+01  
Mg 1.000000e+01 1.424000e+01 2.260000e+01  
Mg 1.210000e+01 1.214000e+01 2.050000e+01  
Mg 1.420000e+01 1.424000e+01 2.260000e+01  
Mg 1.630000e+01 1.214000e+01 2.050000e+01  
Mg 1.840000e+01 1.424000e+01 2.260000e+01  
Mg 2.050000e+01 1.214000e+01 2.050000e+01  
Mg 2.260000e+01 1.424000e+01 2.260000e+01  
Mg 1.000000e+01 1.844000e+01 2.260000e+01  
Mg 1.210000e+01 1.634000e+01 2.050000e+01  
Mg 1.420000e+01 1.844000e+01 2.260000e+01  
Mg 1.630000e+01 1.634000e+01 2.050000e+01  
Mg 1.840000e+01 1.844000e+01 2.260000e+01  
Mg 2.050000e+01 1.634000e+01 2.050000e+01  
Mg 2.260000e+01 1.844000e+01 2.260000e+01  
Mg 1.000000e+01 2.264000e+01 2.260000e+01  
Mg 1.210000e+01 2.054000e+01 2.050000e+01  
Mg 1.420000e+01 2.264000e+01 2.260000e+01  
Mg 1.630000e+01 2.054000e+01 2.050000e+01  
Mg 1.840000e+01 2.264000e+01 2.260000e+01  
Mg 2.050000e+01 2.054000e+01 2.050000e+01  
Mg 2.260000e+01 2.264000e+01 2.260000e+01  
Mg 1.424000e+01 1.421000e+01 3.060000e+01  
Mg 1.844000e+01 1.421000e+01 3.060000e+01  
Mg 1.424000e+01 1.841000e+01 3.060000e+01  
Mg 1.844000e+01 1.841000e+01 3.060000e+01  
Mg 1.424000e+01 1.001000e+01 3.480000e+01

Mg 1.844000e+01 1.001000e+01 3.480000e+01  
Mg 1.004000e+01 1.421000e+01 3.480000e+01  
Mg 1.424000e+01 1.421000e+01 3.480000e+01  
Mg 1.634000e+01 1.211000e+01 3.270000e+01  
Mg 1.844000e+01 1.421000e+01 3.480000e+01  
Mg 2.264000e+01 1.421000e+01 3.480000e+01  
Mg 1.004000e+01 1.841000e+01 3.480000e+01  
Mg 1.214000e+01 1.631000e+01 3.270000e+01  
Mg 1.424000e+01 1.841000e+01 3.480000e+01  
Mg 1.634000e+01 1.631000e+01 3.270000e+01  
Mg 1.844000e+01 1.841000e+01 3.480000e+01  
Mg 2.054000e+01 1.631000e+01 3.270000e+01  
Mg 2.264000e+01 1.841000e+01 3.480000e+01  
Mg 1.424000e+01 2.261000e+01 3.480000e+01  
Mg 1.634000e+01 2.051000e+01 3.270000e+01  
Mg 1.844000e+01 2.261000e+01 3.480000e+01  
Mg 1.424000e+01 1.001000e+01 3.900000e+01  
Mg 1.844000e+01 1.001000e+01 3.900000e+01  
Mg 1.004000e+01 1.421000e+01 3.900000e+01  
Mg 1.214000e+01 1.211000e+01 3.690000e+01  
Mg 1.424000e+01 1.421000e+01 3.900000e+01  
Mg 1.634000e+01 1.211000e+01 3.690000e+01  
Mg 1.844000e+01 1.421000e+01 3.900000e+01  
Mg 2.054000e+01 1.211000e+01 3.690000e+01  
Mg 2.264000e+01 1.421000e+01 3.900000e+01  
Mg 1.004000e+01 1.841000e+01 3.900000e+01  
Mg 1.214000e+01 1.631000e+01 3.690000e+01  
Mg 1.424000e+01 1.841000e+01 3.900000e+01  
Mg 1.634000e+01 1.631000e+01 3.690000e+01  
Mg 1.844000e+01 1.841000e+01 3.900000e+01  
Mg 2.054000e+01 1.631000e+01 3.690000e+01  
Mg 2.264000e+01 1.841000e+01 3.900000e+01  
Mg 1.214000e+01 2.051000e+01 3.690000e+01

Mg	1.424000e+01	2.261000e+01	3.900000e+01
Mg	1.634000e+01	2.051000e+01	3.690000e+01
Mg	1.844000e+01	2.261000e+01	3.900000e+01
Mg	2.054000e+01	2.051000e+01	3.690000e+01
Mg	1.424000e+01	1.421000e+01	4.320000e+01
Mg	1.634000e+01	1.211000e+01	4.110000e+01
Mg	1.844000e+01	1.421000e+01	4.320000e+01
Mg	1.214000e+01	1.631000e+01	4.110000e+01
Mg	1.424000e+01	1.841000e+01	4.320000e+01
Mg	1.634000e+01	1.631000e+01	4.110000e+01
Mg	1.844000e+01	1.841000e+01	4.320000e+01
Mg	2.054000e+01	1.631000e+01	4.110000e+01
Mg	1.634000e+01	2.051000e+01	4.110000e+01

Atomic coordinates (d = 9Å)

Mg	1.000000e+01	1.004000e+01	1.000000e+01
Mg	1.420000e+01	1.004000e+01	1.000000e+01
Mg	1.840000e+01	1.004000e+01	1.000000e+01
Mg	2.260000e+01	1.004000e+01	1.000000e+01
Mg	1.000000e+01	1.424000e+01	1.000000e+01
Mg	1.420000e+01	1.424000e+01	1.000000e+01
Mg	1.840000e+01	1.424000e+01	1.000000e+01
Mg	2.260000e+01	1.424000e+01	1.000000e+01
Mg	1.000000e+01	1.844000e+01	1.000000e+01
Mg	1.420000e+01	1.844000e+01	1.000000e+01
Mg	1.840000e+01	1.844000e+01	1.000000e+01
Mg	2.260000e+01	1.844000e+01	1.000000e+01
Mg	1.000000e+01	2.264000e+01	1.000000e+01
Mg	1.420000e+01	2.264000e+01	1.000000e+01
Mg	1.840000e+01	2.264000e+01	1.000000e+01
Mg	2.260000e+01	2.264000e+01	1.000000e+01
Mg	1.000000e+01	1.004000e+01	1.420000e+01

Mg	1.420000e+01	1.004000e+01	1.420000e+01
Mg	1.840000e+01	1.004000e+01	1.420000e+01
Mg	2.260000e+01	1.004000e+01	1.420000e+01
Mg	1.000000e+01	1.424000e+01	1.420000e+01
Mg	1.210000e+01	1.214000e+01	1.210000e+01
Mg	1.420000e+01	1.424000e+01	1.420000e+01
Mg	1.630000e+01	1.214000e+01	1.210000e+01
Mg	1.840000e+01	1.424000e+01	1.420000e+01
Mg	2.050000e+01	1.214000e+01	1.210000e+01
Mg	2.260000e+01	1.424000e+01	1.420000e+01
Mg	1.000000e+01	1.844000e+01	1.420000e+01
Mg	1.210000e+01	1.634000e+01	1.210000e+01
Mg	1.420000e+01	1.844000e+01	1.420000e+01
Mg	1.630000e+01	1.634000e+01	1.210000e+01
Mg	1.840000e+01	1.844000e+01	1.420000e+01
Mg	2.050000e+01	1.634000e+01	1.210000e+01
Mg	2.260000e+01	1.844000e+01	1.420000e+01
Mg	1.000000e+01	2.264000e+01	1.420000e+01
Mg	1.210000e+01	2.054000e+01	1.210000e+01
Mg	1.420000e+01	2.264000e+01	1.420000e+01
Mg	1.630000e+01	2.054000e+01	1.210000e+01
Mg	1.840000e+01	2.264000e+01	1.420000e+01
Mg	2.050000e+01	2.054000e+01	1.210000e+01
Mg	2.260000e+01	2.264000e+01	1.420000e+01
Mg	1.000000e+01	1.004000e+01	1.840000e+01
Mg	1.420000e+01	1.004000e+01	1.840000e+01
Mg	1.840000e+01	1.004000e+01	1.840000e+01
Mg	2.260000e+01	1.004000e+01	1.840000e+01
Mg	1.000000e+01	1.424000e+01	1.840000e+01
Mg	1.210000e+01	1.214000e+01	1.630000e+01
Mg	1.420000e+01	1.424000e+01	1.840000e+01
Mg	1.630000e+01	1.214000e+01	1.630000e+01
Mg	1.840000e+01	1.424000e+01	1.840000e+01

Mg	2.050000e+01	1.214000e+01	1.630000e+01
Mg	2.260000e+01	1.424000e+01	1.840000e+01
Mg	1.000000e+01	1.844000e+01	1.840000e+01
Mg	1.210000e+01	1.634000e+01	1.630000e+01
Mg	1.420000e+01	1.844000e+01	1.840000e+01
Mg	1.630000e+01	1.634000e+01	1.630000e+01
Mg	1.840000e+01	1.844000e+01	1.840000e+01
Mg	2.050000e+01	1.634000e+01	1.630000e+01
Mg	2.260000e+01	1.844000e+01	1.840000e+01
Mg	1.000000e+01	2.264000e+01	1.840000e+01
Mg	1.210000e+01	2.054000e+01	1.630000e+01
Mg	1.420000e+01	2.264000e+01	1.840000e+01
Mg	1.630000e+01	2.054000e+01	1.630000e+01
Mg	1.840000e+01	2.264000e+01	1.840000e+01
Mg	2.050000e+01	2.054000e+01	1.630000e+01
Mg	2.260000e+01	2.264000e+01	1.840000e+01
Mg	1.000000e+01	1.004000e+01	2.260000e+01
Mg	1.420000e+01	1.004000e+01	2.260000e+01
Mg	1.840000e+01	1.004000e+01	2.260000e+01
Mg	2.260000e+01	1.004000e+01	2.260000e+01
Mg	1.000000e+01	1.424000e+01	2.260000e+01
Mg	1.210000e+01	1.214000e+01	2.050000e+01
Mg	1.420000e+01	1.424000e+01	2.260000e+01
Mg	1.630000e+01	1.214000e+01	2.050000e+01
Mg	1.840000e+01	1.424000e+01	2.260000e+01
Mg	2.050000e+01	1.214000e+01	2.050000e+01
Mg	2.260000e+01	1.424000e+01	2.260000e+01
Mg	1.000000e+01	1.844000e+01	2.260000e+01
Mg	1.210000e+01	1.634000e+01	2.050000e+01
Mg	1.420000e+01	1.844000e+01	2.260000e+01
Mg	1.630000e+01	1.634000e+01	2.050000e+01
Mg	1.840000e+01	1.844000e+01	2.260000e+01
Mg	2.050000e+01	1.634000e+01	2.050000e+01

Mg 2.260000e+01 1.844000e+01 2.260000e+01  
Mg 1.000000e+01 2.264000e+01 2.260000e+01  
Mg 1.210000e+01 2.054000e+01 2.050000e+01  
Mg 1.420000e+01 2.264000e+01 2.260000e+01  
Mg 1.630000e+01 2.054000e+01 2.050000e+01  
Mg 1.840000e+01 2.264000e+01 2.260000e+01  
Mg 2.050000e+01 2.054000e+01 2.050000e+01  
Mg 2.260000e+01 2.264000e+01 2.260000e+01  
Mg 1.424000e+01 1.421000e+01 3.160000e+01  
Mg 1.844000e+01 1.421000e+01 3.160000e+01  
Mg 1.424000e+01 1.841000e+01 3.160000e+01  
Mg 1.844000e+01 1.841000e+01 3.160000e+01  
Mg 1.424000e+01 1.001000e+01 3.580000e+01  
Mg 1.844000e+01 1.001000e+01 3.580000e+01  
Mg 1.004000e+01 1.421000e+01 3.580000e+01  
Mg 1.424000e+01 1.421000e+01 3.580000e+01  
Mg 1.634000e+01 1.211000e+01 3.370000e+01  
Mg 1.844000e+01 1.421000e+01 3.580000e+01  
Mg 2.264000e+01 1.421000e+01 3.580000e+01  
Mg 1.004000e+01 1.841000e+01 3.580000e+01  
Mg 1.214000e+01 1.631000e+01 3.370000e+01  
Mg 1.424000e+01 1.841000e+01 3.580000e+01  
Mg 1.634000e+01 1.631000e+01 3.370000e+01  
Mg 1.844000e+01 1.841000e+01 3.580000e+01  
Mg 2.054000e+01 1.631000e+01 3.370000e+01  
Mg 2.264000e+01 1.841000e+01 3.580000e+01  
Mg 1.424000e+01 2.261000e+01 3.580000e+01  
Mg 1.634000e+01 2.051000e+01 3.370000e+01  
Mg 1.844000e+01 2.261000e+01 3.580000e+01  
Mg 1.424000e+01 1.001000e+01 4.000000e+01  
Mg 1.844000e+01 1.001000e+01 4.000000e+01  
Mg 1.004000e+01 1.421000e+01 4.000000e+01  
Mg 1.214000e+01 1.211000e+01 3.790000e+01

Mg	1.424000e+01	1.421000e+01	4.000000e+01
Mg	1.634000e+01	1.211000e+01	3.790000e+01
Mg	1.844000e+01	1.421000e+01	4.000000e+01
Mg	2.054000e+01	1.211000e+01	3.790000e+01
Mg	2.264000e+01	1.421000e+01	4.000000e+01
Mg	1.004000e+01	1.841000e+01	4.000000e+01
Mg	1.214000e+01	1.631000e+01	3.790000e+01
Mg	1.424000e+01	1.841000e+01	4.000000e+01
Mg	1.634000e+01	1.631000e+01	3.790000e+01
Mg	1.844000e+01	1.841000e+01	4.000000e+01
Mg	2.054000e+01	1.631000e+01	3.790000e+01
Mg	2.264000e+01	1.841000e+01	4.000000e+01
Mg	1.214000e+01	2.051000e+01	3.790000e+01
Mg	1.424000e+01	2.261000e+01	4.000000e+01
Mg	1.634000e+01	2.051000e+01	3.790000e+01
Mg	1.844000e+01	2.261000e+01	4.000000e+01
Mg	2.054000e+01	2.051000e+01	3.790000e+01
Mg	1.424000e+01	1.421000e+01	4.420000e+01
Mg	1.634000e+01	1.211000e+01	4.210000e+01
Mg	1.844000e+01	1.421000e+01	4.420000e+01
Mg	1.214000e+01	1.631000e+01	4.210000e+01
Mg	1.424000e+01	1.841000e+01	4.420000e+01
Mg	1.634000e+01	1.631000e+01	4.210000e+01
Mg	1.844000e+01	1.841000e+01	4.420000e+01
Mg	2.054000e+01	1.631000e+01	4.210000e+01
Mg	1.634000e+01	2.051000e+01	4.210000e+01

Atomic coordinates (d = 10Å)

Mg	1.000000e+01	1.004000e+01	1.000000e+01
Mg	1.420000e+01	1.004000e+01	1.000000e+01
Mg	1.840000e+01	1.004000e+01	1.000000e+01
Mg	2.260000e+01	1.004000e+01	1.000000e+01

Mg	1.000000e+01	1.424000e+01	1.000000e+01
Mg	1.420000e+01	1.424000e+01	1.000000e+01
Mg	1.840000e+01	1.424000e+01	1.000000e+01
Mg	2.260000e+01	1.424000e+01	1.000000e+01
Mg	1.000000e+01	1.844000e+01	1.000000e+01
Mg	1.420000e+01	1.844000e+01	1.000000e+01
Mg	1.840000e+01	1.844000e+01	1.000000e+01
Mg	2.260000e+01	1.844000e+01	1.000000e+01
Mg	1.000000e+01	2.264000e+01	1.000000e+01
Mg	1.420000e+01	2.264000e+01	1.000000e+01
Mg	1.840000e+01	2.264000e+01	1.000000e+01
Mg	2.260000e+01	2.264000e+01	1.000000e+01
Mg	1.000000e+01	1.004000e+01	1.420000e+01
Mg	1.420000e+01	1.004000e+01	1.420000e+01
Mg	1.840000e+01	1.004000e+01	1.420000e+01
Mg	2.260000e+01	1.004000e+01	1.420000e+01
Mg	1.000000e+01	1.424000e+01	1.420000e+01
Mg	1.210000e+01	1.214000e+01	1.210000e+01
Mg	1.420000e+01	1.424000e+01	1.420000e+01
Mg	1.630000e+01	1.214000e+01	1.210000e+01
Mg	1.840000e+01	1.424000e+01	1.420000e+01
Mg	2.050000e+01	1.214000e+01	1.210000e+01
Mg	2.260000e+01	1.424000e+01	1.420000e+01
Mg	1.000000e+01	1.844000e+01	1.420000e+01
Mg	1.210000e+01	1.634000e+01	1.210000e+01
Mg	1.420000e+01	1.844000e+01	1.420000e+01
Mg	1.630000e+01	1.634000e+01	1.210000e+01
Mg	1.840000e+01	1.844000e+01	1.420000e+01
Mg	2.050000e+01	1.634000e+01	1.210000e+01
Mg	2.260000e+01	1.844000e+01	1.420000e+01
Mg	1.000000e+01	2.264000e+01	1.420000e+01
Mg	1.210000e+01	2.054000e+01	1.210000e+01
Mg	1.420000e+01	2.264000e+01	1.420000e+01

Mg	1.630000e+01	2.054000e+01	1.210000e+01
Mg	1.840000e+01	2.264000e+01	1.420000e+01
Mg	2.050000e+01	2.054000e+01	1.210000e+01
Mg	2.260000e+01	2.264000e+01	1.420000e+01
Mg	1.000000e+01	1.004000e+01	1.840000e+01
Mg	1.420000e+01	1.004000e+01	1.840000e+01
Mg	1.840000e+01	1.004000e+01	1.840000e+01
Mg	2.260000e+01	1.004000e+01	1.840000e+01
Mg	1.000000e+01	1.424000e+01	1.840000e+01
Mg	1.210000e+01	1.214000e+01	1.630000e+01
Mg	1.420000e+01	1.424000e+01	1.840000e+01
Mg	1.630000e+01	1.214000e+01	1.630000e+01
Mg	1.840000e+01	1.424000e+01	1.840000e+01
Mg	2.050000e+01	1.214000e+01	1.630000e+01
Mg	2.260000e+01	1.424000e+01	1.840000e+01
Mg	1.000000e+01	1.844000e+01	1.840000e+01
Mg	1.210000e+01	1.634000e+01	1.630000e+01
Mg	1.420000e+01	1.844000e+01	1.840000e+01
Mg	1.630000e+01	1.634000e+01	1.630000e+01
Mg	1.840000e+01	1.844000e+01	1.840000e+01
Mg	2.050000e+01	1.634000e+01	1.630000e+01
Mg	2.260000e+01	1.844000e+01	1.840000e+01
Mg	1.000000e+01	2.264000e+01	1.840000e+01
Mg	1.210000e+01	2.054000e+01	1.630000e+01
Mg	1.420000e+01	2.264000e+01	1.840000e+01
Mg	1.630000e+01	2.054000e+01	1.630000e+01
Mg	1.840000e+01	2.264000e+01	1.840000e+01
Mg	2.050000e+01	2.054000e+01	1.630000e+01
Mg	2.260000e+01	2.264000e+01	1.840000e+01
Mg	1.000000e+01	1.004000e+01	2.260000e+01
Mg	1.420000e+01	1.004000e+01	2.260000e+01
Mg	1.840000e+01	1.004000e+01	2.260000e+01
Mg	2.260000e+01	1.004000e+01	2.260000e+01

Mg	1.000000e+01	1.424000e+01	2.260000e+01
Mg	1.210000e+01	1.214000e+01	2.050000e+01
Mg	1.420000e+01	1.424000e+01	2.260000e+01
Mg	1.630000e+01	1.214000e+01	2.050000e+01
Mg	1.840000e+01	1.424000e+01	2.260000e+01
Mg	2.050000e+01	1.214000e+01	2.050000e+01
Mg	2.260000e+01	1.424000e+01	2.260000e+01
Mg	1.000000e+01	1.844000e+01	2.260000e+01
Mg	1.210000e+01	1.634000e+01	2.050000e+01
Mg	1.420000e+01	1.844000e+01	2.260000e+01
Mg	1.630000e+01	1.634000e+01	2.050000e+01
Mg	1.840000e+01	1.844000e+01	2.260000e+01
Mg	2.050000e+01	1.634000e+01	2.050000e+01
Mg	2.260000e+01	1.844000e+01	2.260000e+01
Mg	1.000000e+01	2.264000e+01	2.260000e+01
Mg	1.210000e+01	2.054000e+01	2.050000e+01
Mg	1.420000e+01	2.264000e+01	2.260000e+01
Mg	1.630000e+01	2.054000e+01	2.050000e+01
Mg	1.840000e+01	2.264000e+01	2.260000e+01
Mg	2.050000e+01	2.054000e+01	2.050000e+01
Mg	2.260000e+01	2.264000e+01	2.260000e+01
Mg	1.424000e+01	1.421000e+01	3.260000e+01
Mg	1.844000e+01	1.421000e+01	3.260000e+01
Mg	1.424000e+01	1.841000e+01	3.260000e+01
Mg	1.844000e+01	1.841000e+01	3.260000e+01
Mg	1.424000e+01	1.001000e+01	3.680000e+01
Mg	1.844000e+01	1.001000e+01	3.680000e+01
Mg	1.004000e+01	1.421000e+01	3.680000e+01
Mg	1.424000e+01	1.421000e+01	3.680000e+01
Mg	1.634000e+01	1.211000e+01	3.470000e+01
Mg	1.844000e+01	1.421000e+01	3.680000e+01
Mg	2.264000e+01	1.421000e+01	3.680000e+01
Mg	1.004000e+01	1.841000e+01	3.680000e+01

Mg 1.214000e+01 1.631000e+01 3.470000e+01  
Mg 1.424000e+01 1.841000e+01 3.680000e+01  
Mg 1.634000e+01 1.631000e+01 3.470000e+01  
Mg 1.844000e+01 1.841000e+01 3.680000e+01  
Mg 2.054000e+01 1.631000e+01 3.470000e+01  
Mg 2.264000e+01 1.841000e+01 3.680000e+01  
Mg 1.424000e+01 2.261000e+01 3.680000e+01  
Mg 1.634000e+01 2.051000e+01 3.470000e+01  
Mg 1.844000e+01 2.261000e+01 3.680000e+01  
Mg 1.424000e+01 1.001000e+01 4.100000e+01  
Mg 1.844000e+01 1.001000e+01 4.100000e+01  
Mg 1.004000e+01 1.421000e+01 4.100000e+01  
Mg 1.214000e+01 1.211000e+01 3.890000e+01  
Mg 1.424000e+01 1.421000e+01 4.100000e+01  
Mg 1.634000e+01 1.211000e+01 3.890000e+01  
Mg 1.844000e+01 1.421000e+01 4.100000e+01  
Mg 2.054000e+01 1.211000e+01 3.890000e+01  
Mg 2.264000e+01 1.421000e+01 4.100000e+01  
Mg 1.004000e+01 1.841000e+01 4.100000e+01  
Mg 1.214000e+01 1.631000e+01 3.890000e+01  
Mg 1.424000e+01 1.841000e+01 4.100000e+01  
Mg 1.634000e+01 1.631000e+01 3.890000e+01  
Mg 1.844000e+01 1.841000e+01 4.100000e+01  
Mg 2.054000e+01 1.631000e+01 3.890000e+01  
Mg 2.264000e+01 1.841000e+01 4.100000e+01  
Mg 1.214000e+01 2.051000e+01 3.890000e+01  
Mg 1.424000e+01 2.261000e+01 4.100000e+01  
Mg 1.634000e+01 2.051000e+01 3.890000e+01  
Mg 1.844000e+01 2.261000e+01 4.100000e+01  
Mg 2.054000e+01 2.051000e+01 3.890000e+01  
Mg 1.424000e+01 1.421000e+01 4.520000e+01  
Mg 1.634000e+01 1.211000e+01 4.310000e+01  
Mg 1.844000e+01 1.421000e+01 4.520000e+01

Mg	1.214000e+01	1.631000e+01	4.310000e+01
Mg	1.424000e+01	1.841000e+01	4.520000e+01
Mg	1.634000e+01	1.631000e+01	4.310000e+01
Mg	1.844000e+01	1.841000e+01	4.520000e+01
Mg	2.054000e+01	1.631000e+01	4.310000e+01
Mg	1.634000e+01	2.051000e+01	4.310000e+01