

The Perfect Fullerene-Like Borospherene I_h -B₂₀ Protected Theoretically by Alkaline Earth Metal: Multi-Layered Spherical Electride Molecules as Electric Field Manipulated Second-Order Nonlinear Optical Switches

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Table S1. The symmetry, bond lengths (B-B, B-Mg, in Å) and diameter of the B₂₀ cage (*d*, in Å) for Mg₁₂&B₂₀ at different calculation levels.

Level	Symmetry	B-B	B-Mg	<i>d</i>
PBE0/6-311G(d)	<i>I</i> _h	1.721	2.388	4.82
PBE0/6-311+G(d)	<i>I</i> _h	1.720	2.387	4.82
TPSSH/6- 311G(d)	<i>I</i> _h	1.725	2.396	4.84
B3LYP/6- 311G(d)	<i>I</i> _h	1.723	2.408	4.83

