Table S1 Single point energies at the MP2/gen level

<table>
<thead>
<tr>
<th></th>
<th>Mg(N₅)₂</th>
<th>Ca(N₅)₂</th>
<th>Sr(N₅)₂</th>
<th>Ba(N₅)₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>-547.02988</td>
<td>-582.52523</td>
<td>-576.41790</td>
<td>-571.22260</td>
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<tr>
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<td>-547.03997</td>
<td>-582.47740</td>
<td>-576.37978</td>
<td>-571.19974</td>
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<tr>
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<td>-582.47741</td>
<td>-576.37975</td>
<td>-571.19973</td>
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<tr>
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<td>-582.47741</td>
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<td>-571.19971</td>
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<tr>
<td>VI</td>
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Table S2 Single point energies at the MP4/gen level*

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<th>Mg(N₅)₂</th>
<th>Ca(N₅)₂</th>
<th>Sr(N₅)₂</th>
<th>Ba(N₅)₂</th>
</tr>
</thead>
<tbody>
<tr>
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<td>-571.22557</td>
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</table>

*Since results obtained at MP4D, MP4DQ, MP4SDQ and MP4SDTQ levels show the same conclusion, only that of MP4D are shown here.
Figure S1 Decomposition paths of Ca(N₃)$_2$, St(N₃)$_2$ and Ba(N₃)$_2$. 