#### Supporting Information

**A sustainable CVD approach for ZrN as potential catalyst for nitrogen reduction reaction.**

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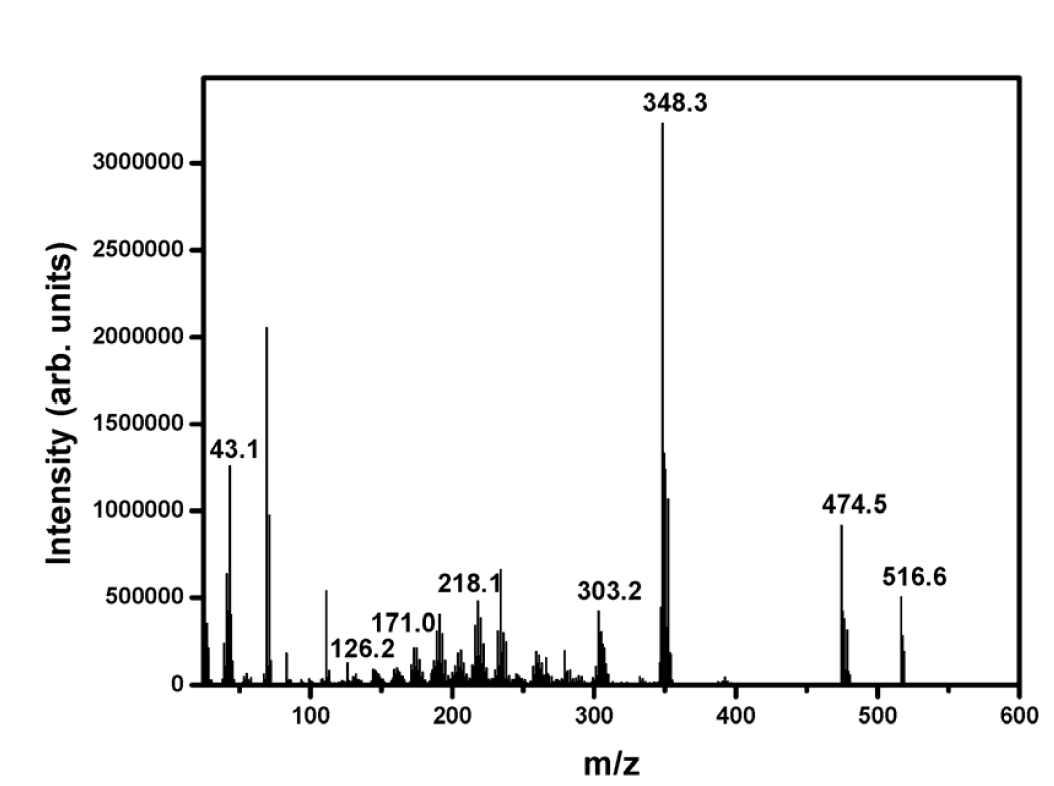
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# Precursor Characterization

## Electron Impact Mass spectrometry (EI-MS)



**Figure S1**. Mass spectrum of [Zr{η2 (*i*PrN)2CNMe2}2(NMe2)2] (**1**). (EI-MS, 70 eV).1

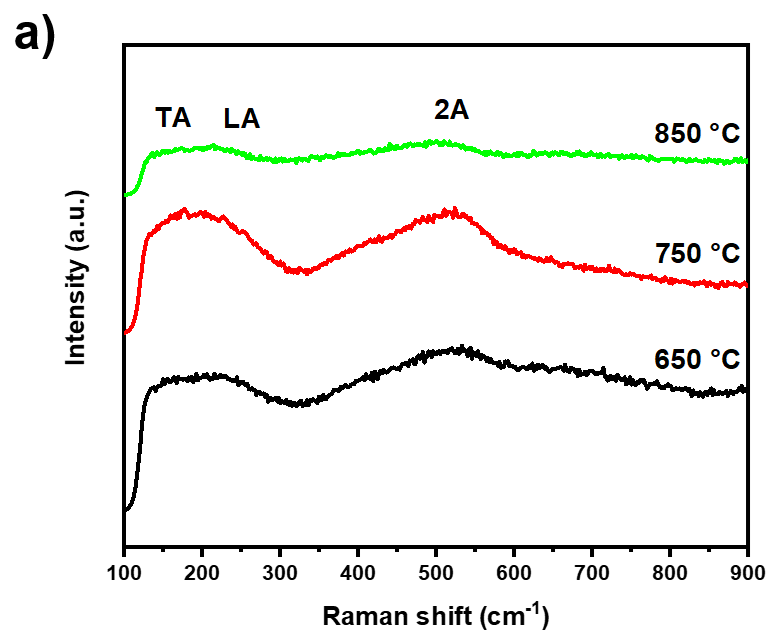
**Table S1**. Proposed EI-MS fragmentation pattern of compound (**1**).

|  |  |  |
| --- | --- | --- |
| Fragments\* | Mass (m/z) | Rel. intensity |
| M+ | 516.6 | 19 |
| M+-NMe2 | 474.5 | 28 |
| M+-NMe2-CDI | 348.3 | 100 |
| M+-NMe2-L | 303.2 | 14 |
| M+-L-CDI | 218.1 | 15 |
| L+ | 171.0 | 4 |
| CDI | 126.2 | 4 |
| NMe2/*i*Pr | 43.1 | 39 |

\*M+ molecular ion; L: {*i*PrN)2CNMe2}; CDI: *N*,*N*´-diisopropylcarbodiimide.

# Thin film analysis

## Raman spectroscopy



**Figure S2**. Raman spectra of ZrN thin films deposited on GC substrates as a function of deposition temperature. The Raman peaks are assigned according to literature reports.2–4

# *Ab initio* molecular dynamics (aiMD)



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